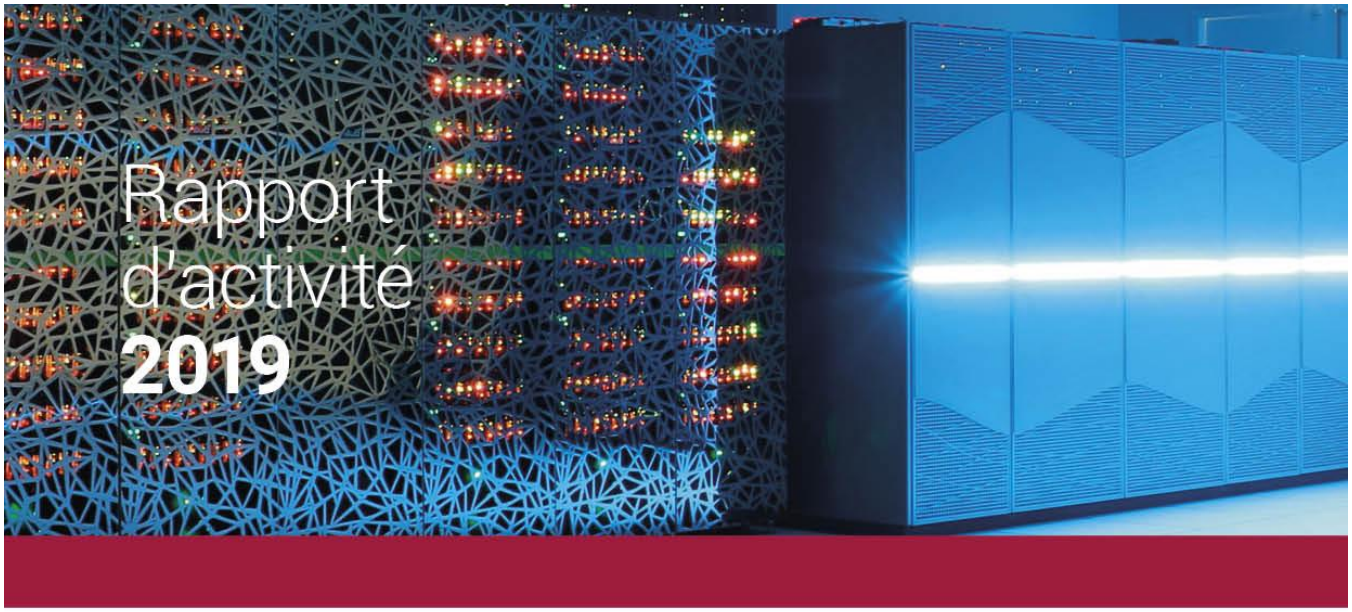


Rapport d'activité **2019**

calmip

INP TOULOUSE

UNIVERSITÉ TOULOUSE III PAUL SABATIER

INSA INSTITUT NATIONAL DES SCIENCES APPLIQUÉES TOULOUSE

isae SUPAERO

cnrs

Université Fédérale Toulouse Midi-Pyrénées

SOMMAIRE

1 Faits marquants

- Vie de l'Unité
  - Janvier 2019 : Arrivée d'un nouvel ingénieur en développement, *Thierry Louge*, personnel CNRS, expert de la valorisation des données
  - Décembre 2019 : Arrivée d'un nouvel administrateur systèmes et réseaux, *Laurent Cabanas*, personnel Université Toulouse III, Paul Sabatier

- Comité d'Attribution :
  - Pour la session d'attribution 2019, le comité d'attribution a examiné : 235 demandes de projets et plus de 136 000 000 heures_cpu demandées

- Ouverture aux entreprises et SiMSEO
  - Quatre projets SiMSEO ont été réalisés
  - Deux nouvelles prestations de service avec des entreprises ont été contractualisées pour réaliser des calculs sur le supercalculateur CALMIP

- Octobre 2019 - Organisation des Journées Calcul et Données **JCAD** en collaboration avec UFTMIP, IRIT et CNES

- Callisto : Développement d'une **interface pour le partage et l'analyse semi-automatique de données**.

- Organisation d'une journée de formation sur le DMP – Data Management Plan

- Cycle de formation spécifique GPU

2 Bilan d'exploitation et d'utilisation 2019 pour la recherche académique

***2019**, en quelques chiffres :*

- **235** projets/dossiers soumis au Comité d'Attribution :
  - **59** nouveaux projets,
  - **176** projets renouvelés.
- **36** laboratoires/unités ayant déposés un projet :
- **747** collaborateurs aux projets dont **290** doctorants ou post-doctorants.
- Attribution de ressources :
  - **136 804 537** heures demandées,
  - **101 766 518** heures attribuées,
  - **81 908 672** heures consommées

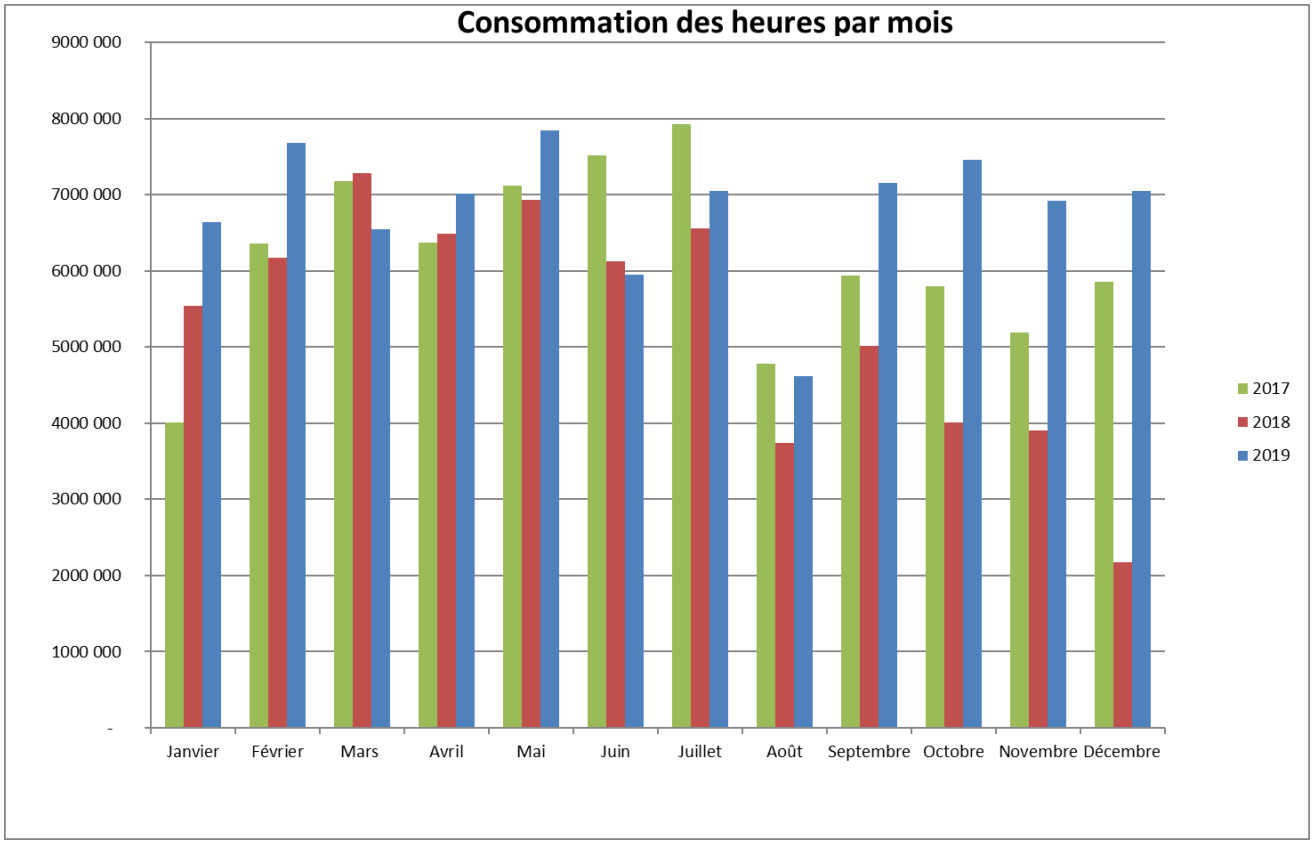


Figure 1 : Consommation par mois des Supercalculateurs Olympe (Sept 2018 -2019) et EOS (2017- Sept 2018)

Par mois la consommation d'Olympe est globalement supérieure à celle d'Eos (2017 = 2 ième année de production). On voit que sur la fin d'année, Olympe a été très utilisée. On retrouve le creux de l'été (possibilité de faire mieux en période estivale). Le niveau de consommation des heures attribuées sur l'ancien Supercalculateur EOS n'a de sens que jusque septembre 2018, date à laquelle le supercalculateur Olympe a été mis en production. La production sur le Supercalculateur Eos a alors été diminuée en conséquence.

2.1 Répartition par thématiques des demandes d'heures de calcul pour la session 2019

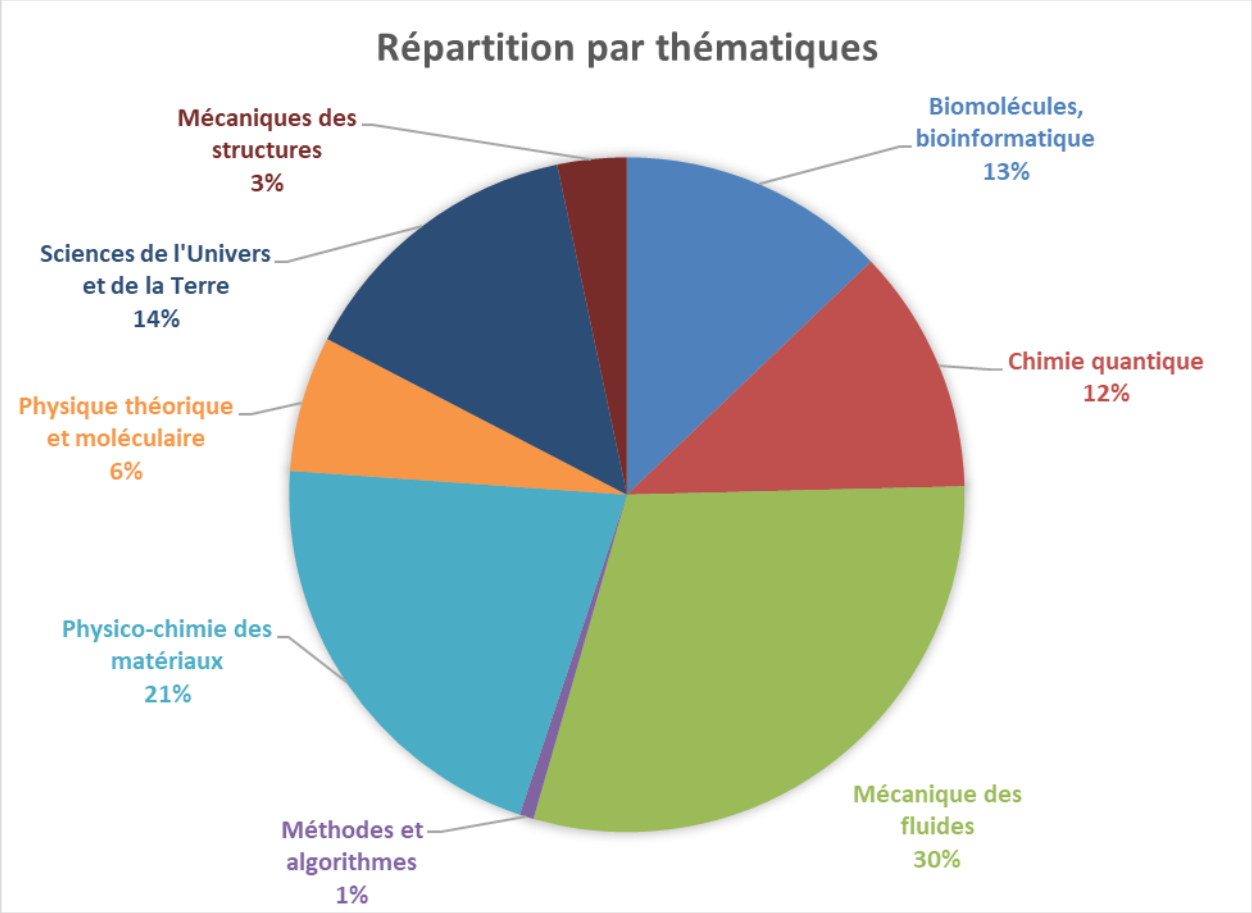


Figure 2 : Répartition des demandes par thématiques pour 2019

La répartition des demandes par thématique reste classique, avec la Mécanique des fluides en tête, suivie de la Physico-chimie des matériaux (Sciences de la Matière), vient ensuite les Sciences de l'Univers et de la Terre et Sciences du Vivant - « Biomolécules – Bioinformatique », puis Chimie Quantique.

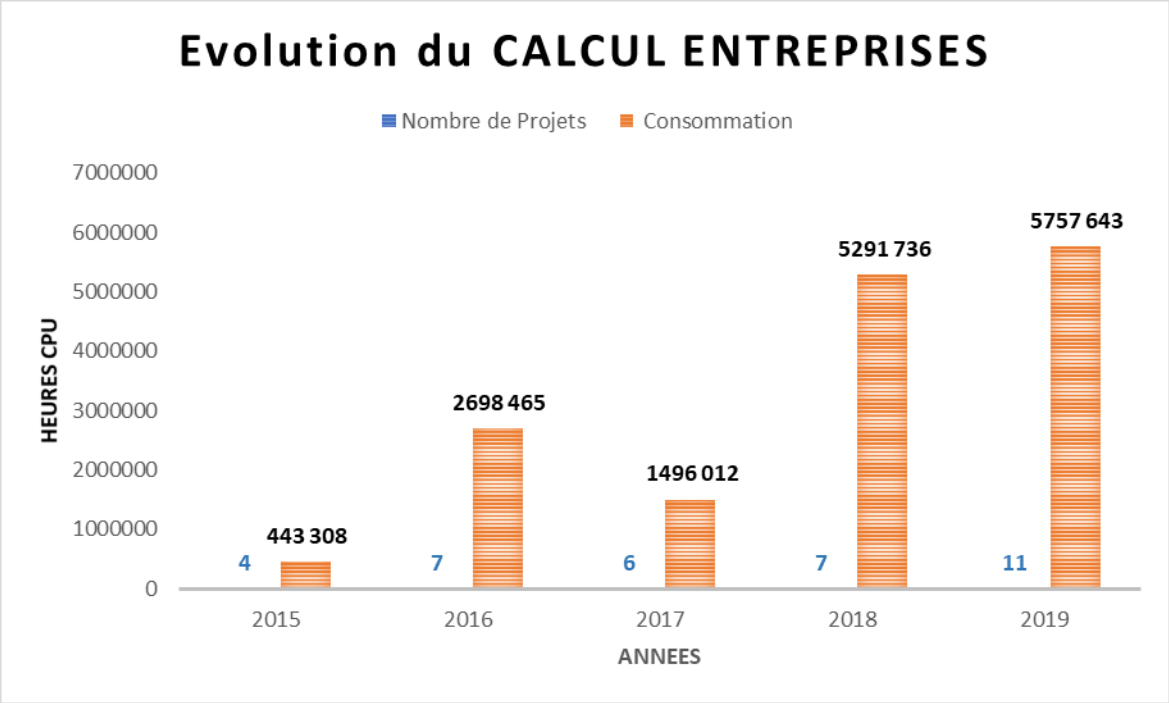
2.2 Ouverture de la plateforme aux entreprises pour des activités d'innovation et de recherche

Dans le cadre du projet Equip@Meso, des entreprises type PME/ETI calculent sur CALMIP, jusqu'à 10% des heures CPU de calcul sont réservées à cette activité.

Leur objectif principal en venant sur CALMIP est d'avoir l'opportunité de collaborer avec des experts HPC et des équipes de recherche, mais aussi de mener des simulations à grande échelle et adapter des méthodes numériques au calcul parallèle.

Sur 2019,

- **11** projets « entreprises » ou projets « test »,
- **5 757 643** heures consommées.



2.3 Formations et animations scientifiques

Formations

→ https://www.calmip.univ-toulouse.fr/spip.php?rubrique15

- **Formation CALMIP : Introduction aux systèmes de Calcul HPC et prise en main du système Olympe**
  - Trois sessions de cette formation ont été proposées : 4 et 5 Février 2019, 7 et 8 Février 2019, 14 et 15 Février 2019
- **Formation ATOS-CALMIP : Prise en main des outils de Debugging et de Profiling ARM**
  - Dates : 12 Juin : Debugging - 13 Juin : Profiling - 14 Juin : application sur les codes utilisateurs
- **Formation GRICAD-CALMIP : Séminaire autour des Données FAIR et des Plans de Management de la Donnée**
  - Date : 27 juin
- **Formation Outils Intel - Inspector - Intel Trace Analyzer - Vector Advisor - Vtune (Amplifier XE)**
  - Dates : 17,18 & 19 Septembre
- **Formation programmation CUDA (2 jours)**
  - Dates : 1er & 2 Octobre 2019
- **Formation programmation OpenACC (2 jours)**
  - Dates : 3 & 4 Octobre 2019
- **Atelier/WorkShop GPU "Dynamique Moléculaire & Physico-chimie des matériaux"**
  - Codes concernés : Amber, Gromacs, Namd, Vasp, Quantum Espresso
  - Dates : 15 & 16 Octobre 2019
- **Formation "Introduction au C++ et à la programmation objet" coorganisée par CALMIP, l'IMFT et le CUTIS**
  - Dates : 5 au 10 Décembre 2019

Animations scientifiques :

- Journée JCAD 2019 – Toulouse : https://jcad2019.sciencesconf.org/
    - Les JCAD 2019 ont été organisées par UFTMIP, CALMIP, IRIT et CNES
    - Présentation du projet CALMIP P19046 - **Portage efficace d'un code de calcul en mécanique des fluides sur GPUs sans coder une ligne de CUDA (ou presque)**
      Annaïg Pedrono [1], Aurélie Louis-Napoléon [1], Pierre Elyakime [1], Maxime PIGOU [1], Mickaël Duval [2], Nicolas RENON [2]
      1 : Institut de mécanique des fluides de Toulouse, Institut National Polytechnique [Toulouse], Université Paul Sabatier, CNRS
      2 : Calcul en Midi-Pyrénées, Institut National Polytechnique [Toulouse], Institut National des Sciences Appliquées - Toulouse, Université Paul Sabatier, PRES Université de Toulouse, CNRS
    - Présentation du projet CALMIP P1440 - **Comparaison de structures anatomiques et calculs intensifs en paléoanthropologie**
      Jean Dumoncel [1], José Braga [1], Emmanuel Courcelle [2], Nicolas Renon [2]
      1 : Anthropobiologie Moléculaire et Imagerie de Synthèse, Université Paul Sabatier, CNRS
      2 : CALMIP, Université Paul Sabatier, Institut National Polytechnique de Toulouse, Institut Supérieur de l'Aéronautique et de l'Espace (ISAE), CNRS, PRES Université de Toulouse
    - Présentation du projet CALMIP - **Calculs de chimie quantique distribués entre méso-centres avec Quantum Package**
      Anthony Scemama [1], Patrick BOUSQUET-MELOU [2], Marie-Sophie Cabot [2], Nicolas Renon [3]
      1 : IRSAMC-Lab. de Chimie et Physique Quantiques, CNRS
      2 : Centre Régional Informatique et d'Applications Numériques de Normandie (CRIANN)
      3 : Calcul en Midi-Pyrénées, Institut National Polytechnique [Toulouse], Institut National des Sciences Appliquées - Toulouse, Université Paul Sabatier, PRES Université de Toulouse, CNRS
    - Présentation du projet CALMIP P12166 - **Application of OpenFOAM on supercomputers to permafrost modeling**
      Laurent Orgogozo [1], Anatoly Prokushkin [2] , Oleg S. Pokrovsky [1], Christophe Grenier [3], Michel Quintard [4], Jerome Viers [1], Stephane Audry [1]
      1 : Géosciences Environnement Toulouse, Institut de Recherche pour le Développement, Université Paul Sabatier, Observatoire Midi-Pyrénées, CNRS
      2 : Sukachev Institute of Forest, Krasnoiarsk, Russie
      3 : Laboratoire des Sciences du Climat et de lÉnvironnement, Université de Versailles Saint-Quentin-en-Yvelines, Commissariat à l'énergie atomique et aux énergies alternatives, Université Paris-Saclay, CNRS
      4 : Institut de mécanique des fluides de Toulouse, Institut National Polytechnique, Université, Paul Sabatier, CNRS

- Présentation du projet CALMIP P19043 - **Utilisation des clusters de calcul en cancérologie : application à l'étude de l'hétérogénéité cellulaire des tumeurs.**
  Frédéric PONT, Pôle technologique du CRCT. Centre de Recherche et de Cancérologie de Toulouse, INSERM UMR1037, Université Toulouse III Paul-Sabatier. ERL 5294 CNRS, Toulouse. Laboratoire d'Excellence Toulouse Cancer, TOUCAN

- **Table ronde " Les Plans de Gestion des Données des projets Scientifiques, quels impacts pour les centres de Calcul et de Données ? "**
  Animation : Nicolas Renon, CALMIP
  Participants : Windpouire-Esther Dzale-Yeumo 1, Emmanuel Courcelle 2, Jean-Yves Nief 3, Jean-Philippe Proux 4, Geneviève Romier 3 5
  1 : INRA
  2 : CALMIP
  3 : CC-IN2P3, CNRS
  4 : GENCI
  5 : France-Grilles (FG-iRODS)

- **CALLISTO : Une interface pour le partage et l'analyse semi-automatique de données.**
  Thierry Louge, orateur Emmanuel Courcelle, Calcul en Midi-Pyrénées, Institut National Polytechnique [Toulouse], Institut National des Sciences Appliquées - Toulouse, Université Paul Sabatier, PRES Université de Toulouse, CNRS

3 Mode d'attribution des ressources de calcul

3.1 Attribution des ressources de calcul pour les académiques

- L'accès aux ressources **CALMIP** est ouvert aux projets validés par le **Comité d'Attribution.** Pour cela, les responsables de projets scientifiques doivent faire une demande d'attribution de ressources informatiques sur GRAMC - **G**estion de **R**essources et **A**ttribution pour **M**éso**C**entre**:** https://attribution-ressources.calmip.univ-toulouse.fr.
- Deux sessions d'examen de dossiers ont lieu dans l'année :
  - une première session principale "A" a lieu à l'automne, pour distribuer des heures de calcul sur la totalité de l'année suivante (1er Jan. —> 31 Déc.),
  - une seconde session complémentaire "B" a lieu au printemps, pour distribuer des heures de calcul non consommées jusqu'à la fin l'année en cours (1er Juill. —> 31 Déc.).
- Une évaluation scientifique est effectuée par les experts du Comité d'Attribution. Ces experts formulent ensuite des recommandations qui permettent d'effectuer des allocations d'heures sur le supercalculateur CALMIP. Les heures attribuées sont gratuites pour les utilisateurs qui sont dans un laboratoire de la COMUE UT (universités, écoles et EPST), financées par les tutelles des laboratoires. **Un rapport d'activité des travaux réalisés est demandé.**

3.2 Attribution des ressources de calcul pour les entreprises

- Après des échanges entre CALMIP et l'entreprise qui souhaite démarrer un projet de calcul, une première réunion est organisée entre l'équipe HPC de l'entreprise qui porte le projet et l'équipe support utilisateurs de CALMIP. L'idée est de bien appréhender côté entreprise le besoin en calcul, les outils numériques utilisés, la problématique algorithmique … et côté CALMIP, de faire une présentation du service proposé aux entreprises.
- Un premier contrat avec un projet test de 5 000 h de calcul (le nombre d'heures peut être adapté au besoin projet) est conclu avec un ou plusieurs comptes spécifiques ouverts sur le calculateur. Ce projet sert à installer le code de l'entreprise et à faire des premiers tests de fonctionnement et de performance. Deux jours d'ingénieur CALMIP sont dédiés en moyenne à la préparation et mise en œuvre de ce type de projet test.
- Si la PME est satisfaite de ses premiers tests, et si elle souhaite poursuivre son projet, il lui sera alors proposé un contrat de prestation de services adapté à ses besoins de calcul.

4 Bilan scientifique, résumé des projets de l'année 2019

4.1 Mécanique des fluides

Test sur le code SBM

Projet démarré en 2019

LGC - Laboratoire de Génie Chimique (UMR 5503)

Porteur de projet : **Irea Touche**

Nous faisons des simulations avec un code écrit en python, utilisant les bibliothèques fipy et pytrilinos pour résoudre des équations différentielles. J'aimerai tester la scalabilité du code pour savoir s'il serait pertinent de demander un projet pour 2019.

MFEED

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Gérald Debenest**

The MFEED platform has been created by the Institut of Fluid Mechanics of Toulouse to study and solve a wide range of problems encountered by companies or public communities. The platform is specialized in the numerical simulations in fluid mechanics and provides services in modeling, analysis, expertise and advices to IMFT's partners. As part of its activities, the platform develop and maintain numerical tools (mainly based on OpenFOAM) which can be used to solve complex and large scale numerical problems requiring high computing capacities. In order to validate these tools, the MFEED platform request some CPU time to test parallel efficiency and result accuracy on the OLYMPE system. Theses tests will also show to the MFEED's industrial partners the potential offered by the OLYMPE supercomputer and may allow to set up collaborations with CALMIP and the Institut of Fluid Mechanics of Toulouse.

Interactions fluide-structure souple : cas des vibrations induites par vortex d'un long cylindre flexible

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Rémi Bourguet**

Flow-structure interactions involving flexible bodies are ubiquitous in nature and engineering systems. They result in structural fatigue but may also be regarded as mechanical energy converter in the context of flow energy harvesting. Vortex-induced vibrations (VIV) are an important class of interaction phenomena which are driven by the synchronization between the motion of the body and the unsteadiness of the flow surrounding it. Real physical systems subjected to VIV generally involve flexible bodies (e.g. marine cables exposed to ocean currents, plants in wind) and thus distributed interaction mechanisms with many degrees of freedom (structural modes). Paradoxically, VIV have been mainly studied through the (over-)simplified case of an elastically-mounted rigid cylinder with one or two degrees of freedom. The present project aims at bridging the gap towards real systems by exploring the physics of VIV for a long flexible cylinder. On the basis of large scale three-dimensional flow-structure simulations, we will propose a combined analysis of the structural responses and flow dynamics, with a particular attention paid to the mechanisms of energy transfer

between the fluid and the moving, deformable body. This numerical study will benefit from joint experimental studies on VIV carried out in collaboration with the Center for Ocean Engineering at MIT and at IMFT.

Combustion dans les milieux divisés : procédés pour réduire les émissions de gaz à effet de serre.

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Enrica Masi**

The goal of this project is to model and study, by the 3D unsteady numerical simulation, two industrial processes that are involved in the reduction of the greenhouse gas emissions. The first one concerns the iron steel industry. The latter has been working for years on strategies to improve its production processes in order to reduce the emissions of carbon dioxide. One of these strategies consists in recycling the steel gases by injecting, after heating and reforming, the hot reducing gas into the blast-furnace nozzles. This involves a modification of the injection parameters that impacts the formation of the blast-furnace cavities. These cavities are crucial as they ensure the right distribution of the reducing gas throughout the coke bed so ensuring the efficiency of the entire process. Their investigation represents the first goal of the present project. The second process is a Chemical Looping Combustion (CLC) using pet-coke as a fuel. CLC has been proved to be an efficient technology for steam generation allowing CO2 capture with no additional cost for gas separation. In this project a theoretical and numerical modeling of the solid-fueled CLC will be developed and used at pilot scale first, and to simulate a CLC prototype at the end. The use of the three-dimensional unsteady numerical simulation will make it possible to study the local and instantaneous behavior of the reactive multiphase flow and to understand the complex interplay of fluid dynamics and reactions occurring in the entire system such that improvements in the reactor design can be suggested.

Collision oblique de deux sphères dans un fluide visqueux

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Laurent Lacaze**

The modelling of the bouncing of two particles evolving in a viscous fluid remains a challenging task. Even if the normal bouncing has been often considered in the literature, the case of an oblique interaction remains an open question. Yet, the full description of a two-particle interaction requires the understanding of the whole fluid contribution, in particular in the tangential direction prior contact. This description can not be reached in experiments as the fluid can play a significant role at a very small gap scale between the two particles. Numerical modelling is therefore the only tool which would allow to reach this goal. Here, we propose a set of numerical simulations coupling an Immersed Boundary Method to solve the fluid phase at the grain scale and a Discrete Element Method for the grains motions, including a spring-dashpot model for the solid contact between the two particles. The solid contact occurs at the surface roughness scale for real grains, which is here linked to the scale imposed by the fluid mesh. For these reasons, modelling the bouncing at a reasonable length scale requires a very fine resolution of the fluid phase, which is estimates here to be of the order of D/100, with D the grain diameter. Several simulations with typical mesh resolution of D/50 and D/100 are proposed in this project. A simulation consists in a sphere falling under gravity in a viscous fluid and interacting with a fixed sphere which is slightly out of alignment with the moving sphere. Different angles of interaction will be considered in order to extract a pertinent model to describe this oblique bouncing.

Estimation des gradients de température pendant les phases de remplissage et vidange de réservoir de gaz. Application aux réservoirs d'hydrogène.

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **David Lo Jacono**

This research project falls within energy mitigation. In order to reduce carbon emissions, hydrogen is one of the paths that are promising. The global market related to hydrogen-fueled tanks is already important and will certainly be more so. This research project deals with the optimal processing of filling and de-filling H2-tanks. Indeed, it is forecasted that before 2030 one out of three vehicles (in western countries) will be hydrogen-fueled. These vehicles will need to be re-filled in H2 within 5mins for an autonomous range of 500km (similar to carbon-based vehicles). Hence, a storage of H2 is required in a highly pressurized manner (700 bar) would be optimal in order to reach these objectives. However, this choice of storage necessitates composite materials in order to achieve light-weight and minimal dimensions goals. Furthermore, at these high pressures, while filling or emptying an increase of temperature is bound to happen (from thermodynamics principles). The composite materials used have a conductivity much small than metals and in a first approach can be thought as an insulator. In turn, the temperature within the tank is higher than those within metal tanks. Safety standards state that the temperature should remain within -40C and +85C at all times. To our knowledge, there are no simple unsteady models that give the temperature gradients as a function of the geometry and the (de)filling rates. Buoyancy effects are to be kept hence precluding any symmetry assumptions. Furthermore, the correct modelling of turbulent mixing is of upmost importance. This project stems from previous work which exhibited large deviations with specific experiments devoted to this project.

Analyse aérothermodynamique de l'intrados d'un corps de rentrée

Projet démarré en 2019

ONERA - Office National d'Etudes et de Recherches Aéronautiques

Porteur de projet: **Philippe Reulet**

The present study is an analysis of steady continuum hypersonic flows with real gas effects in the context of atmospheric reentries. Atmospheric reentries are a real challenge and the European Space Agency needs to get more experience in this domain. For this purpose, the European Space Agency designed an automatic reentry vehicle, called Intermediate eXperimental Vehicle (IXV). The IXV was launched on a suborbital trajectory to recreate the conditions of an atmospheric reentry from the low Earth orbit and gathered data on the hypersonic flow during the flight. ONERA participates to the post-analysis of the temperature and pressure measurements performed inside the IXV thermal protection systems during its mission. The purpose of this study is to improve our understanding on the critical phenomena that occur during an atmospheric reentry: chemical non-equilibrium in the flow, chemical reactions at the surface, thermal non-equilibrium, radiative heat transfers… The purpose of the present demand for the CALMIP supercomputer is to run 3D steady Navier-Stokes simulations of the hypersonic flow around the IXV, in order to study the phenomena in the flow that caused the heating measured inside the thermal protection systems of the IXV windward surface. These 3D Navier-Stokes simulations are prepared using two previous studies: - An estimate of the convective heat flux at the windward surface of the IXV using an inverse heat conduction method, based on temperature measurements performed by thermocouples in the thermal protection systems. This analysis allowed to estimate the convective heat flux that will be compared to the results of 3D simulations. - 1D steady Navier-Stokes simulations, at the IXV stagnation point. Short 1D simulations give us the opportunity to test various models for the phenomena that could occur during a reentry. This study allows us to improve our choices of

the chemical and physical models for the 3D simulations. This study takes place during a PhD thesis, at ONERA – Toulouse Center, which started on October 1st, 2016.

Simulations d'écoulements diphasiques avec le code CEDRE

Projet démarré en 2019

ONERA - Office National d'Etudes et de Recherches Aéronautiques

Porteur de projet: **Julien Troyes**

L'ONERA travaille depuis plusieurs années sur les mécanismes qui pilotent l'atomisation dans les systèmes aérospatiaux. Le rôle d'un système d'atomisation est de produire sur une distance très courte un brouillard de fines gouttelettes de manière à maximiser la surface d'échange entre le liquide et l'écoulement gazeux. Dans plusieurs applications il est nécessaire de pulvériser un liquide. Dans le cadre de la combustion, les motoristes souhaitent assurer l'homogénéisation de la vapeur de carburant et le comburant afin d'optimiser la combustion, et cela en présence des forts débits de carburant nécessaires pour alimenter un turboréacteur. Le phénomène de l'atomisation est aussi utilisé afin de générer des sprays pour d'autres raisons : création de fines couches d'huile dans les systèmes de lubrification, comme système de refroidissement des parois chaudes, pour la création de revêtements ou bien pour l'incrément temporaire de la poussée des moteurs d'avions à hautes performances. Une autre application particulière est la réduction du bruit généré par un jet chaud, comme par exemple les jets de lanceurs spatiaux : une réduction du niveau d'émission sonore peut être réalisée par l'injection d'une pulvérisation d'eau dans le jet chaud supersonique. Le processus d'atomisation est un mécanisme très complexe à simuler en raison de son caractère multi-échelle : plusieurs ordres de grandeur séparent la taille caractéristique de l'injecteur et les plus petites gouttes produites. D'autre part, les instabilités de l'atomisation primaire sont à la base d'un processus de formations des gouttes strictement instationnaire : les oscillations à grande échelle des jets déterminent les zones où les paquets liquides sont crées et pulvérisés et la densité de particules au cours de l'atomisation est élevée. On observe la coexistence locale de grosses et petites structures. Les méthodes de simulation directe sont capables de traiter l'atomisation jusqu'à la taille de la goutte, permettant d'obtenir les caractéristiques du brouillard généré. Cependant, elles ne sont pas applicables à un système d'injection réel en raison de leur coût. D'autre part, les simulations faite à niveau industriel de chambres de combustion négligent les mécanismes de formation du spray : les gouttes sont directement injectées dans le domaine de calcul, la complexité et l'instationnarité du processus d'atomisation n'est pas prise en compte. Une piste pour simuler efficacement le processus complet d'atomisation est le couplage de deux types de modèles, adaptés aux différentes échelles du problème : un premier modèle dit à phases séparées qui permet de reproduire les grandes échelles du phénomène d'atomisation ; un second modèle adapté à la description des brouillards, dit à phase dispersée, qui permet de reproduire le transport et l'évaporation des gouttelettes créées par le processus de fragmentation. Développée au cours de plusieurs thèses ([1], [5]), cette méthodologie prend l'appellation de simulation LSS (« Large Scales Simulation ») dans le cadre de ce projet.

Analyse d'expériences de turbulence de grille

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Matthieu Mercier**

The global estimation for plastic waste in the ocean is about 200 000 pieces/km2, however, it represents only between 2 and 5% of annual global plastic inputs [1]. This implies that current tools are not able to determine correctly neither plastic waste concentration nor their location, especially their vertical distribution. Available

estimates are based on a model proposed by Kukulka et al (2012) taking into account of the distribution plastic waste according to the sea state ([2]) Our objective is to improve the modeling of plastic particles dynamics in the upper ocean turbulence, which depends on the properties of plastic particles and on the coupling with the turbulent flow, with a specific on the smallest plastic particles (smaller than a few millimeters). An experimental approach is realized to provide a parametric modeling of the link between the concentration of plastic with depth and the kinetic turbulent energy profile. Experiments are realized in a rectangular tank with fluid agitation obtained with an oscillating grid near the fluid surface. Plastic particles are tracked optically, and the fluid phase is also observed thanks to small tracers (Particle Image Velocimetry measurements). [1] J.R. Jambeck, R.Geyer, T.P. Siegler, M.Perryman, A.Andrady, R.Narayan and K.L.Law, Plastic waste inputs from land int the ocean , Science, 768, 2015 [2] T.Kukulka, G.Proskurowski and S.Morét-Ferguson, D.Meyer and K.Law, The effect of wind mixing on the vertical distribution of buoyant plastic debris, Geophysical Research Letters, 39, 2012

Simulations LBM pour les écoulements de suspensions

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Eric Climent**

Particulate flow find a vast field of application ranging from chemical reactors, such as fluidized beds, over biomedical scenarios, such as blood flow in arteries, to oil and gas flow in petroleum technology. The Lattice Boltzmann method (LBM) offers an efficient algorithm to calculate four-way coupled particulate flows as direct numerical simulations (DNS). LBM is a relatively new method for numerical fluid simulations. Instead of directly solving the Navier-Stokes equation, we solve the Lattice Boltzmann equations which describe the flow on a mesoscopic level. Macroscopic flow quantities can be retrieved from this scheme and Chapman-Enskog's theory shows that continuity and the NS equation are correctly recovered. There are several advantages of LBM im comparison to traditional Navier Stokes solver. Due to it's Cartesian grid, meshing of complex geometries is straight forward, it's kinetic description on a mesoscopic scale allows simple calculation of momentum transfer and it is well suited for multiphase flows. Most important is the possibility to run efficiently on massively parallel architectures which will be essential in future generation of supercomputers. In this work we want to study a suspended flow over an obstacle to analyze influence of rigid particles on flow characteristics. This involves solving the fluid flow, momentum exchange between fluid and solid phases and particle-particle as well as particle-obstacle collisions. From high resolution DNS we hope to gain a better understanding of hydrodynamic interaction of particulate flow and improve modeling approaches for large scale simulations.

Portage du Code de calcul JADIM sur GPU

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Annaig Pedrono**

JADIM is a research code developed at IMFT (Institut de Mecanique des Fluides de Toulouse, Toulouse, France). This numerical tool solves the 3D unsteady incompressible Navier-Stokes equations on curvilinear orthogonal meshes. The code is based on a finite volume approach using a classical projection method to enforce incompressibility. A second order space and time finite volume method with a structured mesh is used (third order Runge- Kutta scheme for non-linear term resolution coupled with a Crank-Nicolson scheme for the semi-implicit part). JADIM code is parallelized with an approach based on domain decomposition. 80 %

of computation time is spent in the pressure solver which is a pseudo-Poisson system. For a diphasic simulation, matrix coefficients change at each time step and a linear system is solved. We plan to optimize the use of AMGX library developed by Nvidia. We already have done promising tests during the Hackathon GENCI in december 2018 (http://www.genci.fr/fr/node/967). We obtained promising results with a gain between 10 and 20 when we added a NV100 GPU to the CPU. We achieved first tests of openACC directives in a GPU Hackathon in Jülich and managed to run the core of the code on GPU for a monophasic simulation. At present time, JADIM code has been running on 12000 cores for grid size up to one billion grid points. It scales until about 300 nodes. All the results we will obtain in JADIM code could be used in other research code developed in our laboratory. Indeed linear system resolutions are used in a lot of fluid dynamics codes due to incompressibility or implicit schemes. We expect this project permit us to really benefit from GPU computation power.

Relaxation d'un bouchon de colloïdes dans des microcanaux

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Olivier Liot**

The process by which pores become clogged by flow-advected colloid aggregation, as well as their unclogging, is crucial for the industry. The understanding of these mechanisms is indeed central to improve the filtration membranes used in the treatment of water. It is a very current research topic, at the interface of several communities (mechanics, physics, process engineering, chemistry, biology) (Dressaire & Sauret, 2017). Moreover, from a fundamental point of view, the way in which a reversible transport process leads to the formation of partially or completely irreversible structures is of great interest, particularly in the understanding of the physico-chemical interactions between the colloids themselves or with the surfaces. So far, experimental investigations have mainly been conducted with systems where diffusion may be neglected. However, the use of highly Brownian colloids whose characteristic sizes are comparable to physicochemical interaction scales is of great interest both fundamental and applied - because very present in the industry. Recent experimental work has shown that when the hydrodynamic forcing is stopped (stopping the pressure drop forcing the flow), part of the plug is re-suspended in the fluid, while another remains stuck to the walls of the pores. This project aims to experimentally visualize, by fluorescence microscopy, the relaxation dynamics of a highly Brownian colloid plug when forcing is stopped. For this purpose, micro-manufactured model pores are used, according to the recently published approach (Liot et al., 2018). This will provide detailed access to the spatio-temporal dynamics of unclogging. Various parameters can be tuned, such as the Brownian motion of the colloids, the pore inlet shape, the colloid-colloid and colloid-surface interactions, the plug aging, and the hydrodynamic forcing. The study of this dynamic should make it possible to obtain clues on the micro-structure of the clog.

Simulation numérique de poches de gaz en conduite verticale ou faiblement inclinées, pour différentes viscosités de la phase continue

Projet démarré en 2019

TBI - Toulouse Biotechnology Insitute

Porteur de projet: **Alain Line**

The objective of the project is to simulate both the shape and the celerity of isolated gas slugs (Taylor bubble in a vertical pipe and Benjamin bubble in a horizontal or slightly inclined pipe). The simulations will be compared to experimental data acquired during the PhD of Alexandre Boucher (TBI, 2018-2021). The data

concern celerity of gas slugs (by cross-correlation between diodes or by Bubble Image Velocimetry), the shape of the gas slug (by shadowgraphy), the velocity in the liquid phase (by Particle Image Velocimetry). The gas is air ; the liquids are newtonian (water or mixture water-Breox, similar density but viscosity multiplied by 102 or 103). The simulations will first consist 3D visualisations of vertical Taylor bubbles for different liquid viscosity and pipe diameter (assessing the surface tension effects). The general shape, the velocity field around the bubble and the wall and interfacial shear stresses will be analysed. The same analysis will also be conducted for horizontal and slightly inclined pipes (inclination between 0° and 15°). Two type of simulations will be done, the first is a 3D draining pipe experiment and the second is a 3D isolated gas bubble propagation in liquid. The simulations will be performed with Transat code, based on immersed surface technic and level set to catch the gas-liquid interface. It is a highly parallelized code.

Reconstruction bathymétrique par méthides d'apprentissage

Projet démarré en 2019

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Rachid Benshila**

Costal regions are currently facing environmental risks and resource problems, aggravated by demographic pressure and overexploitation. The environmental context of extreme events (floods, coastal erosion) combined with demographic pressure is a limiting factor for the development of coastal regions. In this context, the estimation and monitoring of coastal topography is becoming increasingly critical, while long-term in situ measurements remain difficult and costly. Recently, less expensive alternatives based on video imaging have emerged. They are currently based mainly on trajectory detection of individual pixels to estimate the velocity and dissipation of waves, and invert them to obtain bathymetry. We propose here a brand new approach through different learning algorithms applied to the same video images. We will use synthetic data obtained using a simulator to implement our neural network. In this ideal environment, we will test the use of different layers and self-encoding (selection of significant images) to obtain better accuracy. These results will be compared to the topographies obtained with more traditional methods.

Étude de l'influence des tensioactifs sur le transfert de matière gaz-liquide.

Projet démarré en 2019

LGC - Laboratoire de Génie Chimique (UMR 5503)

Porteur de projet: **Benjamin Lalanne**

This project deals with the study of the influence of surfactants on the gas-liquid mass transfer. In chemical engineering processes such as for wastewater treatment, the mass transfer rate around oxygen bubbles has been shown to be significantly decreased as compared to the same configuration with cleaner water; however, the influence of surfactants is not taken into account in the correlations for transfer predictions. Then, complementary studies both experimentally and numerically are proposed to understand the modification of transfer due to surfactants. Experimentally, optical technics, like the Laser Induced Fluorescence with Inhibition method, are able to visualize the oxygen concentration field around a rising bubble and quantify the transfer rate; here, we propose to couple this method with the use of a fluorescent surfactant so as to gather information on its zones of accumulation. In parallel, direct numerical simulations will be performed with the in-house code DIVA for two-phase flows, which captures the interfaces with the Level-Set method, by considering the problem of mass transfer around a rising bubble, either in the reference situation with clean interfaces (with a perfect slip condition for velocity at the interface) or in the case of interfaces with adsorbed surfactants (inducing discontinuities of viscous stresses due to the Marangoni

effect). In this way, the numerical method is able to follow both the bulk and surface concentration of surfactants, which are coupled through mass exchanges depending on the adsorption and desorption processes, and to simulate the modified hydrodynamics as compared to clean bubbles. Simulations will be employed to conclude if such a change in the velocity field is able to reflect the modification of transfer rate observed in the experiments, at large concentration of surfactants and for bubbles in the inertial regime. A numerical challenge will be to resolve accurately the thin mass boundary layers around the rising bubbles at large Péclet number, requiring the use of parallel computations.

Stabilisation et contrôle de la combustion par injection d'hydrogène

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Laurent Selle**

Stringent regulations on pollutants emissions applied to combustion devices to comply EU objectives, make the development of low-emission combustors a major design challenge for aero and land-based gas turbines. These new designs are usually operated in lean combustion mode conditions limiting NOx emissions but also promoting a resonant coupling between combustion and acoustic modes. These combustion instabilities have many detrimental effects leading in extreme cases to mechanical failure. In this scenario, the combination of hydrogen with standard carbon-based fuels is actually considered one of the most promising technical solution for clean combustion. Lean flame stabilisation is enhanced by hydrogen high flame speeds and a wide flammability range. Furthermore, hydrogen offers no emissions of HC or CO2 and due to lower temperatures NOx emissions decreases significantly. Despite the large number of investigations concerning hydrogen enriched flames, yet few are the studies focusing on the contest of combustion dynamics. The present project aims to fill this gap of knowledge by proposing numerical investigations on a hydrogen enriched swirled flames. This corresponds to experiments carried out on the MIRADAS longitudinal combustor at the IMFT Laboratory operated with a perfectly premixed CH4/Air mixture enriched with hydrogen up to 2% of the total power. This initial phase of the project first focuses on flame stabilisation. The impact of the hydrogen injection on the flame structure and stabilisation mechanisms are investigated by means of large eddy simulations (LES). The high-fidelity compressible Navier-Stokes solver AVBP is coupled with analytically reduced chemistry (ARC) kinetic schemes allowing a detailed description of the chemical reactions. The study is then extended to the analysis of the response of the flames to incoming acoustic perturbations. Starting from the experimental measurements, interesting points of the pure CH4/Air and enriched CH4/Air-H2 flame transfer functions (FTFs) are numerically investigate by submitting the predicted unperturbed flames to an acoustic longitudinal perturbation. For each operative case the FTFs gain and phase are retrieved and the impact of the hydrogen injection on the main flame/acoustic coupling mechanisms is investigated.

Méthodes particulaires LTP pour modélisation convection-diffusion

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Franck Plouraboué**

Je souhaiterai tester un code parallèle MPI particulaire sur une architecture multi-coeurs comprenant un nombre de coeur important. Le code a été testé sur des calculateurs de bureaux de 16 coeurs, mais je voudrais juger comment il se comporte avec un grand nombre de coeurs. Avant de faire une demande plus conséquente, je voudrais d'abord tester et valider le code grâce à ce projet.

Simulation numérique de jets impactants

Projet démarré en 2019

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **David Fabre**

Dans le cadre d'un projet sur les instabilités de jets impactants, en collaboration avec les universités de Berlin et Bayreuth, nous souhaitons faire des tests avec les codes de nos collègues allemands sur les moyens de calcul de Calmip. En cas de succès nous ferons ensuite une demande d'heure plus conséquente pour la session de janvier.

Combustion de particules d'aluminium post-détonation

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Laurent Selle**

After the detonation of an oxygen-deficient homogeneous high explosive, a phase of turbulent combustion, called afterburning, takes place at the interface between the rich detonation products and air. Its modelling is instrumental for the accurate prediction of the performance of these explosives. Because of the high temperature of detonation products, the chemical reactions are mixing-driven. Modelling afterburning thus relies on the precise description of the mixing process inside fireballs. There is an additional complexity when the explosive is heterogeneous, i.e. initially seeded with reactive metallic particles. The after burning of these particles greatly impacts the global energy release but the details of their influence on the flow and the post-detonation phase is still unknown. The overall objective of this study is to address these phenomena via unsteady numerical simulation : DNS and LES. This project is at the center of the PhD work of Jimmy Suarez and the continuation of a collaboration between IMFT and CEA (Gramat) over the past 4 years. A previous PhD (Sebastien Courtiaud) paved the way with numerical simulations of homogeneous explosives and we now tackle the influence of aluminium particles. The unsteady simulations aim at understanding the underlying mechanisms of aluminium combustion under such extreme conditions and assessing their influence on the post-detonation processes. On the practical side, the detailed simulations guide the development of low-order models that are routinely used at CEA. The key ingredients of the numerical method are (1) a compressible solver with detailed combustion models and (2) a lagrangian tracking of the particles. The solver is the AVBP code, jointly developed by Cerfacs and IFPEN.

Etude des phénomènes instationnaires appliqués aux machines tournantes

Projet démarré en 2018

ISAE/DAEP - Département Aérodynamique, énergétique et propulsion

Porteur de projet: **Yannick Bousquet**

This project aims to analyse the impact of unsteady effects on the performance of axial and radial turbomachinery components. Due to the environmental issues in the aviation domain, engineers have to design more and more efficient components. It is today wheel known that the further rise of efficiency will occur from a good comprehension of unsteady mechanisms and by taking them into consideration during the design procedure. There are many sources of unsteadiness in turbomachinery components. There can be naturally segregated in two categories. The first one considers unsteady effects which are periodic in time and then linked to the blade passing frequency. Interaction mechanisms between rotor and stator fall in this category. The second category concerns unsteady effects which are not linked to the blade passing frequency

and includes phenomena such as rotating stall and surge. This project aims to better understand both, the unsteady mechanisms correlated and uncorrelated to the blade passing frequency. It is divided in five sub-project. The first one concerns the analysis of the stall inception process in a high speed centrifugal compressor. The second one evaluates the impacts of an inlet flow distortion on the stability limit for an axial fan. The third one focuses also on the impacts of an inlet flow distortion but consider an integrated rotor for distributed propulsion application. The fourth one aims to study unsteady mechanisms uncorrelated to the blade passing frequency in an axial fan operating at highly loaded windmilling conditions. Finally, the last project concerns the analysis of unsteady flow field in a variable geometry radial turbine having a rotor with splitter blades.

Dernières publications:

- Benichou, E., Dufour, G., Bousquet, Y., Binder, N., Ortolan, A., & Carbonneau, X. (2019). Body force modeling of the aerodynamics of a low-speed fan under distorted inflow. - **doi:** pu.doi **url:** pu.open_url

SIMULATION NUMERIQUE DIRECTE DES PROCESSUS D'ATOMISATION

Projet démarré en 2018

ONERA - Office National d'Etudes et de Recherches Aéronautiques

Porteur de projet: **Jean-Luc ESTIVALEZES**

This project focuses on the direct simulation of the atomization of a liquid phase in two different cases. The first concerns the impact of Supercooled Large Droplets on aircraft wings, which can lead to ice formation elsewhere than in protected areas. Since the deposit rate resulting from this type of impact is not well known, for a better understanding of this phenomenon, a direct simulation numerical approach has been chosen. This study will focus on the mechanisms of impact and the emission of secondary drops (splashing). Indeed, this numerical approach allows access to phenomena that are difficult to capture experimentally, such as characteristic times generally lower than the microsecond and the characteristic lengths of the order of a micrometer. The second concerns the modeling of the assisted primary atomization of fuel. No model is able today to predict the characteristics of the spray atomization air-blast. A fundamental objective of this study is to provide information and data to build and validate models, which would predict the initial characteristics of the spray in a large scale approach. To this end, this project proposes to carry out several direct numerical simulations of assisted atomization on a simplified but relevant configuration, ie a plane liquid layer sheared by a gas flow in a periodic domain.

Dernières publications:

- Toward direct simulation of high speed droplet impact, T. Xavier, D. Zuzio, J.L. Estivalèzes, Meccanica, P1-16, 2019 - **doi:** pu.doi
- DNS simulation and analysis of periodic planar liquid sheet assisted atomization, M. Averseng, D. Zuzio, A. Boutsikakis, J.l. Estivalezes, ICMF2019, Mai 2019 -

Granular rheology in turbulent bedload transport

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Raphael Maurin**

Considering a granular bed submitted to a surface fluid flow, bedload transport is classically defined by opposition to suspended load as the part of the grains entrained close to the bed. Turbulent bedload transport

has been extensively studied with regard to its importance for earth surface processes such as natural riverbed morphological evolution. Despite a century of modern research on the subject, turbulent bedload transport understanding remains limited, and predictions can lead to sediment transport rate up to three orders of magnitude different from what is observed in the field. In this framework, it is important to study the underlying physical mechanisms associated to turbulent bedload transport, in order to strengthen the phenomenon understanding and increase the prediction capabilities for engineering purposes. To do so, we consider simulations of idealised steady uniform configurations of turbulent bedload transport with monodisperse spherical particles. The description of each independent particle with a discrete element method, coupled with a 1D volume-averaged fluid resolution, enable us to analyze precisely the granular behavior and characterize the associated mechanisms. The goal of the present project is to analyze the granular rheology in turbulent bedload transport focusing on the transition from dense to dilute granular behavior. This transition is of importance for the modelling of turbulent bedload transport in the framework of Euler-Euler models, and represents a major challenge in the description of granular media.

Study of the response of unsteady heat transfer on cross-flow cylinders to acoustical velocity perturbations

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Benoit Bedat**

The objective of the project concerns the unsteady heat transfer of a single or an array of cross-flow cylinder. Simulations are performed to understand and qualify the influence of periodic incoming flow on unsteady heat transfer. This study is performed in parallel with an experiment on thermo-acoustics at IMFT (Rijke tube). It is known that this set up will conduct to thermo-acoustic instabilities when the unsteady heat release exhibits a delay with the acoustical velocity and overcomes the acoustical power lost at the extremities. The heating grid design corresponds to a side by side set-up [4]. In this configuration no wake interactions with another heating elements are possible. Single wire stability computations [5] with a King model [2, 3] leads to the upper regime even for low intensity while the experiment shows another behavior. The King model corresponds to a quasi-stationary response with a single wire with classical correlation for the heat transfer. In order to elucidate, a numerical study of the response of a single wire or an array of wires is performed with valuable parameters (bulk velocity, wire temperature) and with a dilatable formulation of Navier Stokes equations with variable physical properties.

Simulation numérique d'un panache de bulles en fluides visqueux

Projet démarré en 2018

TBI - Toulouse Biotechnology Insitute

Porteur de projet: **Alain Line**

The objective of the project renewal is to continue to simulate the hydrodynamics, mixing and mass transfer induced by a bubble plume. The simulations gave good results; additional work is needed to compare simulations to experimental data acquired during the PhD of David Laupsien (LISBP, December 8th 2017). The first results will be presented during the second International Workshop in Hamburg, June 2018, « Non-Invasive Experimental Tools and Numerical Methods for the Investigation of Non-Reactive and Reactive Gas-Liquid Flows ». As a reminder, the data bank concerns the frequencies of the bubble plume oscillation, the liquid velocity fields (mean flow, periodic motion and turbulence), bubble characteristics (distributions of sizes and shapes, velocities) and gas fraction distributions for ellipsoidal bubbles and spherical caps. The simulations are performed with NEPTUNE CFD code. Eulerian model for dispersed bubbly flow is tested in order to improve

the modelling of interfacial transfer of momentum and pseudo-turbulence induced by the bubbles. During the next semester, different large scale models (LIM, large interface model, GLIM, generalized large interface model and LBM large bubble model) will be tested (LIM, GLIM and LBM) in the case of spherical caps plumes in viscous fluids and compared to our data. Depending on these models, different mesh sizes are required, implying different mesh sensitivity tests. In addition, the physical time is large since the plume oscillation period is of order of 30 seconds and time averaging requires at least 10 periods of time. Thus, the resource demand is high.

PNM

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Marc Prat**

Drying of porous media is central to many environmental and engineering applications. In this context, this project aims at performing a major breakthrough in the modelling of the drying process in capillary porous media from a combination of state of the art pore network modelling (PNM) and pore network simulations. Two- and three-equation continuum models will be developed taking into account the non-local equilibrium condition of the vapour and from the distinction between the percolating and non-percolating liquid clusters. The secondary capillary structures corresponding to the liquid trapped in various geometrical singularities of the pore space will be characterised from numerical simulations and will be taken into account as a distinct and specific phase in the continuum models. The pore network models will be developed so as to perform high performance computing (HPC) simulations, which is necessary to meet the length scale separation constraints allowing the computation of continuum model parameters from pore network simulations. A major objective is thus to develop HPC versions of the PNM drying codes.

Simulation Numérique Directe de l'interaction entre la Turbulence et un Changement de phase liquide-vapeur

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Sébastien Tanguy**

The proposed research is a multidisciplinary project at the frontier between Fluid Mechanics, Heat and Mass Transfer at a liquid–gas interface, Applied Mathematics and Scientific Computing. My previous research has contributed to demonstrating the ability and the potential of interface capturing methods, such as Level Set, Ghost Fluid and Volume of Fluid methods, for performing Direct Numerical Simulations in many configurations involving two-phase flows. Many new applications may now be considered, especially in the context of the following two emerging topics: turbulent two-phase flows and liquid-vapor phase change. The proposed research builds upon several current and future collaborations with funding research institutes and industrial partners. We will conclude this short introduction by noting that important progress on this topic may be expected during the next decade due to the previous advances in the field of numerical methods for the simulation of two-phase flows. The new version of the DIVA code may be a leading tool to achieve this result. Especially the recent endeavors devoted to parallel computations with the BlackBox MultiGrid solver will be of great interest to achieve this part of the research project. The important endeavor provided in our recent works on the development and the implementation of numerical methods for two-phase flows is close to reach a sufficient maturity to consider a step forward for my research activities, which will be mainly focused during the next years on more practical applications. All these developments have been integrated in a single

and upgraded version of the numerical code DIVA (Dynamics of Interface for Vaporization and Atomization), benefiting of a much more efficient structure (parallel computations for all the solvers, BlackBox MultiGrid, improved WENO scheme for the Level Set method, turbulent inflow generator) than the previous versions in order to push back the current limits of two-phase flows simulations.

Dernières publications:

- A. Urbano, S. Tanguy, G. Huber, C. Colin. Direct numerical simulation of nucleate boiling in micro-layer regime. International Journal of Heat and Mass Transfer 123 (2018) 1128–1137 - **doi:** pu.doi
- Annagrazia Orazzo, Sébastien Tanguy, Direct numerical simulations of droplet condensation, International Journal of Heat and Mass Transfer 129 (2019) 432–448 - **doi:** pu.doi

Control and optimization strategies to improve the aerodynamic performance of complex vehicles

Projet démarré en 2017

ISAE/DAEP - Département Aérodynamique, énergétique et propulsion

Porteur de projet: **Stéphane Jamme**

This project gathers the different numerical studies that are planned to be conducted by our team on the topic of controlling and/or optimizing complex aerodynamic configurations. We mainly focus our work around the following problems: 1. optimizing the mixing between fuel (hydrogen) and oxidizer (air) in the frame of supersonic combustion applications such as the one found in scramjets. This challenge is of fundamental importance both in terms of fuel consumption and pollutant emissions. In that context, we aim at assessing a new idea based on the use of impulsive hydrodynamic instabilities such as Richtmyer-Meshkov instability (RMI) in order to promote the mixing between the species ; 2. developing innovative active flow control strategies, based on synthetic pulsed jets, also referred as ZNMF for Zero Net Mass Flux, to mitigate the flow separation induced by UHBR (Ultra High Bypass ratio) powerplant installation on the suction side of the wing when the aircraft is operated at high angle of attack and low speed. This topic is led in the framework of the Cleansky 2, European Commission funded research program.

Dernières publications:

- R. Messahel, Y. Bury, J. Bodart and N. Doué. Steady and Unsteady compressible Reduced-Order Models of a Zero-Net Mass-Flux Synthetic Jet Actuator. AIAA Aviation Forum, Dallas, USA, 2019. - **url:** pu.open_url
- M. Rasteiro Dos Santos, Y. Bury, P. Graumer and S. Jamme. Can a starting vortex boost the turbulent transition of a Richtmyer-Meshkov instability-induced air/helium mixing zone? 32nd International Symposium on Shock Waves, Singapore, 2019. - **url:** pu.open_url

Numerical simulation of vertically stratified flows past a settling sphere

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Jacques Magnaudet**

The present project deals with the study of the dynamics of a sphere moving vertically in a linearly stratified fluid. Such flows, in which the densities are inhomogeneous, are encountered in many natural configurations (oceans, atmosphere, storage basins, etc.), and can influence the aggregation and migration of particles such as plankton for instance (MacIntyre et al. 1995}. Therefore, as a basic model, it is a topic of great interest to study the dynamics of a sphere in such flows, as well as the wake structures behind it in such a stratified

environment. The dynamics of this type of flow can be characterized by three non-dimensional parameters, namely the Reynolds number, the Froude number, and the Prandtl number. We consider this problem in the context of the Boussinesq approximation, where the influence of the changes in density on the velocity field is limited to the gravity source in the Navier-Stokes equations; the evolution of the density is governed by an advection-diffusion model. It is now well understood that when a sphere moves vertically in a stably stratified fluid, the wake structure behind it collapses from a near-body structure with attached axisymmetric vortices to a far-wake structure which looks like a jet, in which the velocity can be larger than the speed of the sphere. By means of experiments, it has been observed that the jet structure can be very different depending on the flow parameters (Re, Fr,Pr),; see Hanazaki (2009a). However, the physics of the growth of these different types of three-dimensional wakes/jet structures is not clear. Experimental measurements to access three-dimensional flow structures for both the velocity and the density fields remain a great challenge. Regarding the numerical simulations tackling this problem, because the density boundary layer is very thin (about 5. 10^{-3} the sphere radius for salt stratification with Pr=700), very refined meshes are needed close to the sphere and most of the available numerical works focus on axisymmetric simulations (Torres 2000, Hanazaki 2009b), which cannot cover the situations where wake/jet instability happens. Furthermore, global balances on the sphere, such as the drag/lift force exerted by the flow owing to stratification have not been fully investigated (Yick 2009, Doostmohammadi 2014a} especially in the moderate-Re regimes, and for any values of the Prandtl number. This is a point of great importance in the aim of predicting the sphere dynamics. Therefore, the goal of the present project is to: (i) study the evolution process of the wake/jet structures when the dimensionless parameters are changed, typically 1< Re< 300, 0< Fr< infty and 0.7< Pr< 700; (ii) study the physics of these evolutions when Re, Fr and Pr are varied separately; (iii) establish a correlation between the drag coefficient and the dimensionless parameters, namely C_D=f(Re,Fr,Pr), to determine the variation of the drag force when the stratification of the fluid is changed (no such correlation exists nowadays).

Dernières publications:

- J. Zhang, M. Mercier & J. Magnaudet. Unraveling the mechanims of drag enhancement of bodies settling in a stratified fluid. Phys. Rev. Lett. (submitted) –
-

Simulation numérique directe d'écoulements turbulents gaz-particules à l'échelle mesoscopique

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Enrica Masi**

Particle-laden flows in dilute or kinetic regime are encountered in several industrial applications as, for example, in combustion chambers using pulverized coal as fuel for combustion or in circulating fluidized bed. In these flows, particle dispersion plays an important role and requires an accurate modeling. In the last years, several experimental and numerical studies have highlighted the important role of the dispersion and of the preferential concentration in particle-laden turbulent flows. It has been shown, for example, that the velocities of neighboring weakly inertial particles are strongly correlated in space, due to the local interaction with the same fluid turbulence. On the other hand, the velocities of close inertial particles are spatially uncorrelated due to the memory they retain of the interactions with the fluid flow at distances comparable to or greater than the spatial integral scale of the turbulence. Taking into account the particle velocity correlation is very important in the statistical modeling of the particle-particle interactions, in particular in order to correctly model the inter particle collision time. As for the dynamics, the effects due to the particulate inertia have a great impact on the thermal statistical properties of a non-isothermal dispersed phase, such as the temperature variance or the heat flux transported by the agitation. The characterization of the temperature of the particles is crucial in the modeling of the dispersed phase reactive flows. It therefore represents one of the goals of this project. The second goal is the characterization of the influence of the

collisions on the dispersion of particles in turbulent flow. Indeed, in dispersed-phase turbulent flows, collisions can play an important role on the distribution of particles and on the flow dynamics, even for relatively low volume fractions, typically on the order of 0.1%. This influence results from the fact that, on the one hand, collisions between particles reduce the mean free path of the particles and thus modify the dispersion of clouds of solid particles and, on the other hand, collisions induce a phenomenon of redistribution of particles, which can play a major role in the highly anisotropic regions close the walls. A detailed study of these effects is therefore needed in order to better understand the role of collisions, for example close to the wall, and thus to improve the modeling of dispersed phase flows.

Lattice Boltzmann Simulation for aerodynamics in rotating geometries (LaBoSAGe)

Projet démarré en 2017

ISAE/DAEP - Département Aérodynamique, énergétique et propulsion

Porteur de projet: **Nicolas Gourdain**

The most popular method to simulate flows in complex geometries (aircraft, drones, etc.) is the Navier-Stokes approach. With the increase in computing power, Large Eddy Simulation (LES) emerges as a promising technique to improve both knowledge of complex physics and reliability of flow solver predictions. Unfortunately, the computing cost and the difficulty to represent the real geometry still limit its applicability to engineering applications. In that regard, the use of a Lattice-Boltzmann based flow solver can help to overcome these difficulties. While mesh generation is time consuming for Navier-Stokes flow solvers (due to the "body fitted" approach), this step is usually straightforward with a Lattice-Boltzmann Method. Indeed, the method is based on a Cartesian mesh to avoid building a body-fitted mesh around the provided geometry. Instead, the boundaries are represented through off-lattice boundary schemes, and a match between the Cartesian fluid grid and the curved geometry profile is obtained through adequate interpolation. From 2015 to 2018, the Dpt. of Aerodynamics, Energetics and Propulsion of ISAE-Supaero started to develop [1] and bench LES-LBM for micro-air vehicles [2-3]. The software considered at DAEP is the open-source flow solver Palabos, mainly developed by the University of Geneva. The code has been tested on EOS, showing a speedup efficiency of 80% with 1600 cores with a 1,000,000 cells grid [2], representing a full contra-rotating shrouded rotor. In 2018, some fluid/structure interactions capabilities have been implemented in the LBM code. Such FSI are now the target of the project in 2019.

Dernières publications:

- A. Alguacil, T. Jardin and N. Gourdain (2019). Fluid-Structure Interactions and unsteady kinematics of a low-Reynolds number rotor, AIAA J., - **doi:** pu.doi
- N. Gourdain, A. Alguacil and T. Jardin. (2019). Aerodynamic and aero-acoustics performance of unsteady kinematics applied to a rotor operating at low-Reynolds number, 5th symposium on Fluid-Structure Interactions and Control, Crete, Greece -

Dynamique de bulles en présence de surfactants

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Dominique Legendre**

The present study aims at exploring the complex dynamics of bubbles in liquids containing surfactants. In particular, the influence of surfactant on the bubble dynamics in different configuration is studied. These

include the motion of confined and unconfined bubbles in microchanels, the bouncing dynamics of bubbles under free surfaces and the draining of liquid film between a bubble and a free surface or a solid substrate.

Dernières publications:

- O. Atasi, B. Haut, A. Pedrono, B. Scheid, D. Legendre, (2018). Influence of Soluble Surfactants and Deformation on the Dynamics of Centered Bubbles in Cylindrical Microchannel. Langmuir 34 (34) 10048-10062. - **doi:** pu.doi
- G. Rage, O. Atasi, M. M. Wilhelmus, J. F. Hernández-Sánchez, B. Haut, B. Scheid, D. Legendre, R. Zenit, (2018). Bubbles determine the amount of alcohol in Mezcal. arxiv - **doi:** pu.doi

Développement de CPIV

Projet démarré en 2016

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Pierre Elyakime**

La vélocimétrie par images de particules (PIV) est une technique expérimentale de mesure laser non intrusive de champs de vitesse d'écoulements distribués. Cette technique est très utilisé en tant qu'outil expérimental dans la recherche moderne sur la dynamique des fluides, appliquée aux écoulements liquides, gazeux et multiphasiques. CPIV-IMFT est le logiciel de traitement des données issues de la PIV développé au sein de l'Institut de Mécanique des Fluides de Toulouse (IMFT). Il se base sur un algorithme itératif multi grille avec déformation des images. C'est un logiciel multi plateforme, open source, parallélisé et porté sur les supercalculateurs du méso centre de calcul de Midi-Pyrénées EOS et OLYMPE. Ses performances HPC, dépendantes du nombre de nœuds utilisés, permettent aux expérimentateurs de traiter leurs données en temps réel et d'avoir une analyse des données pendant la phase d'expérimentation. L'accélération la plus importante mesurée est d'environ 3000 pour un calcul sur 90 nœuds du supercalculateur OLYMPE. La courbe de speed up montre une accélération linéaire proche de la courbe idéale. CPIV-IMFT est un code écrit en C/C++ et utilise la librairie Open Source de traitement d'images OpenCV ainsi que la librairie MPI. Particle Image Velocimetry (PIV) is an experimental technique for non-intrusive laser measurement of distributed flow velocity fields. This technique is widely used as an experimental tool in modern fluid dynamics research applied to liquid, gaseous and multiphase flows. CPIV-IMFT is the software for processing PIV data developed by the Institut de Mécanique des Fluides de Toulouse (IMFT). It is based on a multi-grid iterative algorithm with image distortion. It is a multiplatform, open source, parallelized and focused software on the supercomputers of the meso computing center of Midi-Pyrénées EOS and OLYMPE. Its HPC performance, depending on the number of nodes used, allows experimenters to process their data in real time and to have an analysis of the data during the experiment phase. The most important acceleration measured is about 3000 for a 90 node calculation of the OLYMPE supercomputer. The speed up curve shows a linear acceleration close to the ideal curve. Its HPC performance allows experimenters to process data very quickly for near real-time data analysis during the experiment phase. CPIV-IMFT is a code written in C/C++ and uses the Open Source image processing library OpenCV as well as the MPI library.

Dernières publications:

- N. Simiriotis et al., Morphing of a supercritical wing by means of trailing edge deformation and vibration at high Reynolds numbers : Experimental and numerical investigation, Journal of Fluids and Structures -
- Experimental study of the boundary layer structure in very shallow flows over a rough bed Loïc Chagot, Frédéric Y. Moulin, Pierre Elyakime and Olivier Eiff -

Drop motion on solid surface

Projet démarré en 2015

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Dominique Legendre**

The present study aims to explore the complex dynamics of the motion of drop on solid surface. In particular we want to address problems controlled by the dynamic of the contact line. Two situations will be considered: a liquid drop spreading after its contact with a solid surface and a drop sliding on an inclined surface. Liquid drop spreading is a challenging subject that has been studied in countless works and its difficulty to simulate is famous because of the triple line problem and the difficulties rising when trying to simulate its movement. Associated to this phenomena, a new theoretical publication predicts the existence of a series of vortices (Moffat Vortices), induced by the movement of the triple contact line which we pretend to study numerically since they have not yet be seen experimentally. Concerning drop sliding on inclined plate, we aim to consider the case of pearling drop that have been observed experimentally and reproduced in numerical simulation for the first time using JADIM during the PhD of Marco Maglio.

Dernières publications:

- M. Febres, D. Legendre. Enhancement of a 2D front-tracking algorithm with a non-uniform distribution of Lagrangian markers Author links open overlay panel. J. of Computational Physics. Volume 358, 2018, p173-200 - **doi:** pu.doi
- H. Si Hadj Mohand, H. Hoang, G. Galliero, D. Legendre 2019 On the use of a friction model in a Volume of Fluid solver for the simulation of dynamic contact lines, J. of Comput. Physics, 93, 29-45. -

Ecoulements raréfiés dans les microactionneurs fluidiques

Projet démarré en 2015

ICA - Institut Clément Ader

Porteur de projet: **Lucien Baldas**

Gas flows in microsystems are of great interest for various applications that touch almost every industrial field. This multi-disciplinary nature and diverse range of application is typified through the following examples: • fluidic micro-actuators for active control of gas flows, from vacuum to high pressure level; • vacuum generators and pumps for extraction or insertion of biological samples; • micro heat exchangers for the cooling of electronic components, chemical applications, energy generation, waste heat recovery and efficiency improvement; • microsystems for mixing or separation for local gas analysis (e.g. monitoring of air quality); Recently, many studies have been devoted to the analysis of gas flows through microchannels. Modelling gas microflows necessitates taking several characteristic length scales into account, such as the mean free path of the molecules and the internal dimensions of microsystems. The ratio between these two characteristic scales, called the Knudsen number, is relatively large in microsystems and the flow is, in many cases, consequently rarefied. This causes local thermodynamic disequilibria and statistical fluctuations of the flow parameters, which represent the main difficulties for the flow modelling. This project is organized in two main axis: Development of fluidic micro-actuators for flow control: The active flow control is a research field in broad expansion. Its main objective is the improvement of vehicles aerodynamics by modifying, by means of actuators, the flow in the boundary layer. The objective is here to design efficient fluidic micro-oscillators which will be used for controlling flow separation over a ramp. This will be done through a numerical study of the influence of various geometrical and operation parameters on the oscillator performances (frequency and jet velocity), taking into account 3D and rarefaction effects. Development of Knudsen micro-pumps: In rarefied gases, flows can be generated by a tangential temperature gradient along a wall without any initial pressure

gradient. This well-known phenomenon is the so-called thermal creep, or thermal transpiration, effect. It is the basis of the Knudsen pump operation principle, which allows gas pumping without any moving part when the gas is under rarefied conditions. This part of the project will be devoted to the numerical design and optimization of original Knudsen pumps consisting of two facing isothermal ratchet carved surfaces with different temperatures.

Dernières publications:

- G. Tatsios, D. Valougeorgis, J. Chen, L. Baldas, S. Colin and S. Stefanov. Parametrization study of the thermally driven rarefied flow between saw-tooth like surfaces. Proceedings of 5th Micro and Nano Flows Conference, Milano, Italy 2016 -
- G. Saliba, L. Baldas, V. Raimbault, A. Batikh, R. Gilblas, St. Orieux, S. Colin, Y. LeMaoult, Study and development of fluidic oscillators for heat removal, International Symposium on Thermal Effects in Gas flows In Microscale – ISTEGIM 2019, Ettlingen, Germany, October 24-25, 2019 - **url:** pu.open_url

Dynamique des courants de gravité de configurations complexes

Projet démarré en 2015

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Thomas Bonometti**

The present project deals with fluid mechanics phenomena. The subject of the project is the study of the dynamics of gravity currents of arbitrary density ratio spreading in complex configurations. Such flows are encountered in many natural configurations (submarine currents flowing along the continental shelf slope, diapirs rising in the Earth crust). While gravity currents dynamics is relatively well understood in situation where inertia is dominant (high Reynolds number flows), the case of currents evolving in highly viscous flows such as those encountered in the upper lithosphere or in volcano conduits still raise open questions. The goal of the present project is to analyze local phenomena inaccessible to laboratory experiments and in-situ measurements with the use of a numerical approach capable of simulation gravity currents of arbitrary density ratio in configuration in the case of highly viscous fluids. This project is done in collaboration with (1) Muriel Gerbault, Olivier Vanderhaeghe, Roland Martin (GET, Toulouse) and (2) Jacques Magnaudet. In the first project, we will cover a wide range of parameters (density ratio, viscosity ratio, Archimedes number, Buoyancy number) in order to assess the transition between a so-called convection regime from a diapirism regime. In the second project, we will analyze the effect of density ratio and initial shape of the interface on the dynamics of viscous exchange flows.

Dernières publications:

- Zgheib N., Bonometti T. & Balachandar S., Suspension-driven gravity surges on horizontal surfaces : effect of the initial shape. Comput. Fluids, 158, 84-95 (2017). - **doi:** pu.doi **url:** pu.open_url
- Salinas J., Bonometti T., Ungarish M. & Cantero M., Rotating planar gravity currents at moderate Rossby numbers : fully-resolved simulations and shallow-water modeling J. Fluid Mech. 867, 114-145
- (2019). - **doi:** pu.doi **url:** pu.open_url

Modélisation et simulation numérique directe de particules complètement résolues

Projet démarré en 2015

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Enrica Masi**

The goal of the project is to improve the understanding of momentum and heat transfer in poly-disperse flows also in the presence of non-spherical particles, in order to model realistic non-isothermal/reactive dense particle-laden flows on the basis of fully-resolved particle direct numerical simulations. Simulations with thousands particles in several dense configurations will be carried out using a Lagrangian VOF tensorial penalty method implemented in THETIS code developed in collaboration with I2M at Université de Bordeaux (Brandle de Motta, 2013, Vincent et al. 2014).

Dernières publications:

- M.-A. Chadil, S. Vincent, J.-L. Estivalèzes, "Accurate estimate of drag forces using particle-resolved direct numerical simulations", Acta Mechanica (2018) - **doi:** pu.doi
- M.-A. Chadil, S. Vincent, J.-L. Estivalezes, "Novel method to compute drag force and heat transfer for motions around sphere", Thermodynamics of Interfaces and Fluid Mechanics (2018) - **doi:** pu.doi

BrainMicroFlow

Projet démarré en 2015

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Sylvie Lorthois**

The morphological, topological and functional study of cerebral microcirculation is a topic of growing interest in the communities of both vascular physiology and neuroimaging. In particular, cerebral blood flow control and diseased-induced modifications at the scale of the vascular network are crucial and unanswered questions. In this context, the development of innovative, cutting edge numerical tools are needed. IMFT is internationally recognized for its work on brain microcirculation modeling (ERC Consolidator Grant BrainMicroFlow #615102 awarded to S.Lorthois). In particular, a new code BrainMicroFlow has been developed, allowing the numerical simulation of blood flow in the cerebro-vascular network. The challenge is now to develop and incorporate mass transfers models (for oxygen, nutrients, tracers). To this end, several tools have been developed with the goal to make a link between the small scale where vessels are individually resolved and larger scales: 1) a 3D-FEM approach solving the advection/diffusion equations has been implemented and is used to check the validity of reduced models 2) a 1D network/boundary element approach, that we recently extended to transient states. The diffusion equation in the brain tissue is solved through integration of Green functions on the boundaries of the capillaries. Then, considering that the capillaries are axisymmetric, the problem is reduced to a pointwize problem along the cylinder axis. 3) a 3D homogenized model of advection/diffusion equation as also been developed, using the volume averaging method. This method allows to take into account the micro-structure of the network to derive effective properties (diffusion coefficients, sources, velocities). These different models will allow us to perform at the same time simulation of blood flow and mass transfers on geometries with total volumes reaching the full human brain scale.

Dernières publications:

- Berg, M; Bracko, O; Davit, Y; Quintard, M; Nishimura, N; Schaffer, CB; Lorthois, S. A new model for molecule exchange in the brain microvascular system: consequences of capillary occlusions in alzheimers disease. JOURNAL OF CEREBRAL BLOOD FLOW AND METABOLISM Meeting Abstract: PB02-E09 Volume: 39 Pages: 301-302 Supplement: 1 (Juilliet 2019) -
- Berg, M., Davit, Y., Quintard, M., Lorthois, S., 2020. Modelling solute transport in the brain microcirculation: is it really well mixed inside the blood vessels? J. Fluid Mech. 884, A39. - **doi:** pu.doi **url:** pu.open_url

Large eddy simulation of complex aerodynamic configurations

Projet démarré en 2014

ISAE/DAEP - Département Aérodynamique, énergétique et propulsion
Porteur de projet: **Julien Bodart**

In our team we mainly focus on turbulent flows applied to external aerodynamics, using Computational Fluid Dynamics and large eddy simulation specifically. We divide this year our demand in three (A-B-C) contributions. We also use eos to run preliminary computations for our current allocation at GENCI (Occigen, Turing) and PRACE (Juqueen) for different kind of problems. Recent developments in the solver include spectral schemes that exhibit optimal accuracy and performance for large scale simulation of turbulent flows. This numerical work will support several of our research topics in which high order schemes are mandatory, together with the legacy finite volume formulation. In this project, we work on the first part (A) which addresses the noise prediction of supersonic jets interaction(collaboration with LMFA). In the second part (B) we are investigating accuracy of complex rotor stator intercation using sliding interfaces. Finally, the last part of the project (C) aim at studying the flow inside jet actuators within a larger flow control study (Cleansky project XPulse).

Dernières publications:

- Romain Gojon, Christophe Bogey, Effects of the angle of impact on the aeroacoustic feedback mechanism in supersonic impinging planar jets, IJA, vol 18, No 2-3 - **doi:** pu.doi **url:** pu.open_url
- Dumon Jéromine, Gourdain Nicolas, Bury Yannick and Michel, Laurent, Fluid-structure interaction between a composite aileron and a turbulent flow at transonic conditions. (2018) In: 53rd 3AF International Conference on Applied Aerodynamics, 26 - 28 March 2018 (Salon de Provence, France). - **url:** pu.open_url

Détermination de propriétés physiques de milieux poreux

Projet démarré en 2013

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Gérald Debenest**

This project aims to study the numerical determination of transport properties of real porous media. This is a complex subject related to fluid mechanics in tortuous geometries at a small scale and very demanding in terms of computations. Thanks to the developments of advanced visualization techniques (microtomography, microscopy), we are now able to obtain at a small scale a real image of the porous medium. The following step is now to use these data to determine the real properties of porous media in terms of permeability, conductivity and effective diffusion. To do so, we need to calculate flow and concentration field at the local scale and then, solve closure problems in periodic cells. This will give us the estimates of larger scale coefficients we could use to represent the transport phenomena. For real media, the challenge consists to find a way to determine effective properties without any influence of boundary values. This year is really devoted to multiphase flow and then to the development of new solvers able to treat the physics at all scale, i.e. microscopic or macroscopic.

Dernières publications:

- Guibert R., Nazarova M., Horgue P., Hamon G., Creux P., Debenest G., (2015) Computational permeability determination from pore-scale imaging: sample size, mesh and method sensitivities, TiPM -

- Horgue, P., Soulaine, C., Franc, J., Guibert, R., & Debenest, G. (2015). An open-source toolbox for multiphase flow in porous media. Computer Physics Communications, 187, 217-226. -

Interaction fluide-structure d'un cylindre en rotation.

Projet démarré en 2012

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **David Lo Jacono**

Vortex-induced vibration (VIV) are of fundamental and practical importance. Indeed, the interactions between a structure within a flow are encountered in many engineering problems. The coupling between the solid and the fluid becomes of prime importance when the former has a natural frequency comparable to the typical frequency of the detached eddies that could occur behind those structures. One can imagine the disastrous impact if both those frequencies become similar (lock-in). On a fundamental viewpoint the strong coupling between the solid and the fluid is a canonical problem where one can study the interaction phenomena between the body and the fluid, including the mechanisms of energy transfer. Here, in this study we are interested in the particular response of the coupled fluid-structure system when one force a steady rotation on a solid (drill pipe in offshore stations) within a uniform flow. The symmetry breaking that the rotation imposes on the equations might lead to a new class of solutions that will be of interest within the VIV and more generally within the bluff body flow community.

Dernières publications:

- Three-dimensional mode selection of the flow past a rotating and inline oscillating cylinder, D. Lo Jacono, R. Bourguet, M. Thompson & J. Leontini, Journal of Fluid Mechanics, 855, 2018 -
- Flow-induced vibrations of a rotating cylinder in an arbitrary plane, R. Bourguet, Journal of Fluid Mechanics, 860:739-766, 2019 -

Simulation et assimilation de données d'écoulements à surface libre en géophysique

Projet démarré en 2012

IMT - Institut de Mathématiques de Toulouse (UMR 5219)

Porteur de projet: **Frédéric Couderc**

This project is mainly focus on parallel numerical simulations of free surface geophysical flows considering unstructured grids. The numerical environment is fully developed at the Toulouse Mathematics Institute in Fortran 2008. At the top level, a library named FUnMesh has been developed with advanced structures to consider unstructured meshes with particular attention to sequential performance and in context of distributed parallel computing (using only the MPI library for the moment). If main activity is to design new models and numerical schemes, it is crucial to test these models and numerical schemes in "real" context with large computations for geophysical flows (time scales implying very large number of time steps). The numerical environment includes several software's applications: - Tolosa: resolving the multilayer shallow water equations using original explicit and semi-implicit Finite Volume schemes with low Froude asymptotic consistency property on collocated or staggered unstructured grids. Main application is coastal oceanography in collaboration with the SHOM under a research contract. - Mingus: resolving original shallow water type models considering surface tension developed in the laboratory under hyperbolic time step restriction, and so avoiding the surface tension one. Applications are industrial film flows with eventually wet/dry fronts in collaboration with ONERA and LIMSI. - Monk: resolving the multifluid compressible Navier-Stokes equations using an original Finite Volume scheme with low Mach asymptotic consistency property as an original implicit

surface tension treatment adding a new transported variable. Main application for the moment is again film flow in collaboration with LIMSI with possibility to test with in future wave breaking for our SHOM activities.

Dernières publications:

- An explicit asymptotic preserving low Froude scheme for the multilayer shallow water model with density stratification. - **doi:** pu.doi **url:** pu.open_url
- Augmented Skew-Symetric System for Shallow-Water System with Surface Tension Allowing Large Gradient of Density - **url:** pu.open_url

imulation numérique de lits fluidisés réactifs gaz-solides

Projet démarré en 2011

LGC - Laboratoire de Génie Chimique (UMR 5503)

Porteur de projet: **Renaud Ansart**

LGC and IMFT, in the frame of the Fermat Research Federation and in collaboration with PROMES laboratory, Institut Français du Pétrole,... are working on the development of mathematical modelisation and numerical simulation of hydrodynamic and transfers in reactive gas-particle fluidized beds. The complexity of involved physical phenomena (interparticle collisions, aggregate formation, evaporation, heat transfer, chemical reaction, ...) and realistic three-dimensional geometries (biomass gasification plants, concentrating solar power plants) lead to use powerful computer resources such as SGI Altix ICE 8200. Simulations are carried out using an Eulerian n-fluid modeling approach for turbulent and polydispersed fluid-particle flows, which is developped and implemented by IMFT (Institut de Mécanique des Fluides de Toulouse) in a specific version of the NEPTUNE_CFD software, known as NEPTUNE_CFD V1.08@Tlse. NEPTUNE_CFD is a multiphase flow software developed in the framework of the NEPTUNE project, financially supported by CEA (Commissariat à l'Énergie Atomique), EDF (Électricité de France), IRSN (Institut de Radioprotection et de Sûreté Nucléaire) and AREVA-NP. The code solves, for each phase, Eulerian three-dimensional unsteady equations of mass, momentum and enthalpy, coupled through the terms of transfer between phases and transport equation of a variable number of scalars. Parallel simulation efficiency of NEPTUNE_CFD has been tested on many platforms Linux PC, supercomputer (SGI ALTIX ICE, NEC, clusters based on AMD Shangaï and Barcelona). Access to source code programs enables the possibility to modify existing models and also to test the build options to improve the performance of the code. Moreover, excellent parallel performances of the code enable the implementation of multiphysics calculation of flows in real flow configurations. One first objective of the projet is the comparison between experimental measurements realised in the LGC and numerical results from the code NEPTUNE_CFD. The aim of the research is the modeling of the coupling between hydrodynamic, and heat and mass transfer to account for additional mechanism such as radiative transfer and chemical reaction in gaz-solid flow.

Dernières publications:

- H. Benoit, R. Ansart, H. Neau, P. Garcia Triñanes, G. Flamant, O. Simonin, 3D numerical simulation of upflow bubbling fluidized bed in opaque tube under high flux solar heating. AIChE Journal. - **doi:** pu.doi **url:** pu.open_url
- F. Sabatier, R. Ansart, H. Zhang, J. Baeyens, O Simonin. Experiments support simulations by the NEPTUNE_CFD code in an Upflow Bubbling Fluidized Bed reactor. Chemical Engineering Journal, in Press. - **doi:** pu.doi

Modélisation du transport sédimentaire par une approche de simulation numérique locale

Projet démarré en 2010

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Laurent Lacaze**

Physical mechanisms involving solid particles and fluid flow are still poorly described due to the lack of knowledge in the local characterization and thus modelling of solid-liquid and solid-solid interactions. However, these local processes play a fundamental role at larger scales such as sediment transport encountered in many natural flows for which environmental impacts become of major societal concern. Erosion and accretion are two important processes involved in these natural issues. The impacts of granular transport can, in fact, be encountered at different scales and applications, ranging from the process industries to landslides and avalanches. In this proposal, we will focus our attention on the environmental context of river, coastal flows, as well as natural hazard such as subaerial or submarine landslides. The objective of this proposal is to provide a better understanding of the physical processes involved in the transport of solid particles, induced by gravity or flow entrainment, at the scale of the grains, via the development of adapted numerical tools. The aim of these numerical methods is the modelling and quantification of such physical processes. The key objective of the numerical strategy proposed here is the ability to resolve interactions between the solid and liquid phases at the scale of the grains, which are critical in coastal and river flows. To this end, we plan to develop two different numerical tools which can be viewed as complementary by virtue of the type of interaction each method can accurately capture (solid-solid vs. fluid-solid).

Dernières publications:

- Izard E., Bonometti T. and Lacaze L. 2014 Modelling the dynamics of a sphere approaching and bouncing on a wall in a viscous fluid. J. Fluid Mech., 747, p. 422—446 - **doi:** pu.doi **url:** pu.open_url
- Izard E., Lacaze L., Bonometti T. & Pedrono A. Numerical modeling of a granular collapse immersed in a viscous fluid. Advances in Hydroinformatics, Springer, Singapore, 1099-1116 (2018). - **doi:** pu.doi

Propriétés de transport des écoulements inertiels de suspension

Projet démarré en 2010

LGC - Laboratoire de Génie Chimique (UMR 5503)

Porteur de projet: **Micheline Abbas**

La plupart des procédés industriels impliquent un écoulement de milieux divisés. Il est important d'en comprendre les propriétés de transport, dans plusieurs domaines d'ingénierie (génie pétrolier, génie de la réaction chimique ou génie agro-alimentaire). En fonction de l'inertie de l'écoulement, de la fraction volumique de la phase solide, de la taille des particules par rapport à la taille de la conduite et aux structures de l'écoulement, du rapport de densité particule/fluide, la présence des particules peut altérer le transfert de quantité de mouvement. Ce projet vise, par l'intermédiaire de la simulation locale, à étudier la dépendance de la dynamique de la suspension sur tous les paramètres déjà énumérés. Par dynamique je sous-entends la modification des propriétés de l'écoulement par la phase dispersée et/ou structuration (ou organisation) de la phase dispersée due à l'écoulement.

Dernières publications:

- Wang, G., Abbas, M., Yu, Z., Pedrono, A., & Climent, E. (2018). Transport of finite-size particles in a turbulent Couette flow: The effect of particle shape and inertia. International Journal of Multiphase Flow, 107, 168-181. - **doi:** pu.doi
- Wang, G., Abbas, M., Pedrono, A., & Climent, E. (2019). Non Spherical and Inertial Particles in Couette Turbulent Large Scale Structures. In Turbulent Cascades II (pp. 197-204). Springer, Cham. -

Modèles de la dynamique des bulles pour la simulation des grandes échelles des écoulements turbulents

Projet démarré en 2009

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Rémi Zamansky**

Bubbly flows (consisting of a continuous liquid phase and a dispersed gas phase) are of great importance for many industrial applications, which include chemical reactors, water treatment (flotation, oxidation, ..), steam generators, drag reduction system or some CO2 capture devices. In these situations, the Reynolds number is usually large and the complexity of such a flow lies in the coupling between the various physical phenomena involved. When the Reynolds number of the flow is very large, the liquid present turbulent fluctuations on the scale of the bubble. Moreover, the large number of bubbles in the flow may induce hydrodynamic interactions between bubbles and can also cause a significant alteration of the carrier phase. Our goal is to propose an approach to perform Large Eddy Simulation (LES) for this kind of two-phase flows. The realistic description of the bubbles dispersion as well as their influence on the continuous phase requires to compute the hydrodynamic forces on the bubbles. These depend on the relative speed of the bubble and the local fluid acceleration. And since these two quantities are mainly set by the small (unresolved) scales of the flow, the LES approach remains challenging. The question is therefore to estimate correctly the turbulent liquid fluctuations at subgrid scales and particular those "seen" by the bubble. This is our motivation for introducing a stochastic modeling of the flow at unresolved scales. The advantage of the approach of coupling LES with stochastic models at subgridscale is to give access to the unresolved intermittent structures of the flow, while taking into account the large scale organization of the flow. The project aims to devise stochastic models representing the bubble/liquid and the bubbles/bubbles interactions at subgrid scales. These models should be based on theoretical and experimental knowledge of the Lagrangian acceleration properties of high Reynolds number turbulent flows. Contributions from the coupling of the LES with a subgrid stochastic modeling for bubbly flows will be studied by comparison with Direct Numerical Simulations (DNS), experimental results and with standard LES.

Dernières publications:

- S. Renaudi`ere de Vaux, R. Zamansky, W. Bergez, P. Tordjeman, and J.-F. Haquet. Destabilization of a liquid metal by nonuniform joule heating. Phys. Rev. E, 96:033103, Sep 2017. - **doi:** pu.doi
- [1] Z. Zhang, D. Legendre, and R. Zamansky. Model for the dynamics of micro-bubbles in high reynolds number flows. Journal of Fluid Mechanics, 879:554–578, 2019. - **doi:** pu.doi

Sensibilité et contrôle des écoulements par simulations numériques h-p

Projet démarré en 2008

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Christophe Airiau**

The present work is associated to the new RTRA STAE project 3C2T (2018-2021) about the control of the turbulent and transitional compressible boundary layer. The three partners (IMFT, CERFACS, ONERA) will build together a new numerical common suite (plateforme) in which high order h-p simulations, based on DNS, LES and Euler equations will be coupled with their discrete adjoint counter part to solve sensitivities, control and optimisation of flows around complex geometry in a large range of Mach number and Reynolds number regimes. At the beginning, and more especifically, the work will concern the control of the instabilities in the transitional flow or of the small scale structures in the turbulent boundary layer flow, in the subsonic and hypersonic regime. The main numerical simulation tool is the recent JAGUAR code developped at CERFACS, in which Discontinuous Galerkin scheme with Spectral Difference are implemented, optimized and validated for HPC purpose. The Adjoint version of each approach will be developped and implemented at IMFT, in collaboration with the partners using the discrete adjoint formulation, but in respect with the scheme

consistancy and the numerical discretization. After a first validated implementation of JAGUAR on OLYMPE and a first simple sensitivity analysis on a double periodic shear layer, the year 2019, will be dedicated to the first implementation of the adjoint DNS, its validation by comparing with existing solution (for instance ASIA and adjoind ASIA, a 2D compressible code ever developped inside this CALMIP project in the periode 2008-2014, and with a local spectral code). The discrete adjoint will be carefully semi-manually implemented, with a code of automatic differentiation in order to supervise and qualify each step of the process (TAPENADE, INRIA). Some additional test cases will be discussed with the ONERA and CERFACS partners.

Dernières publications:

- Rona, A. ; Monti, M ; Airiau, C. On the generation of the mean velocity profile for turbulent boundary layers with pressure gradients under equilibrium conditions, The Aeronautical Journal, (16), N° 1180, 569 -597, - **doi:** pu.doi
- Spagnoli, B ; Airiau, C. Adjoint analysis for noise control in a two-dimensional compressible mixing layer. COMPUTERS & FLUIDS, 37(4), 475-486, - **doi:** pu.doi

Simulation numérique de l'hydrodynamique et des transferts dans les réacteurs gaz-particules à lit fluidisé

Projet démarré en 2001

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Pascal Fede**

Since 2006, IMFT work on the development of mathematical modelling and numerical simulation of hydrodynamic and transfers in reactive gas-particle fluidized beds. The complexity of involved physical phenomena (inter-particle collisions, aggregate formation, evaporation, heat transfer, chemical reaction, ...) and realistic three-dimensional geometries (catalyst injection zone in polymerization reactor, cyclone separator) requires large computer resources. Simulations are carried out using an Eulerian n-fluid modeling approach for turbulent and polydispersed fluid-particle flows, which is developed and implemented by IMFT (Institut de Mécanique des Fluides de Toulouse) in NEPTUNE_CFD. NEPTUNE_CFD is a multiphase flow software developed in the framework of the NEPTUNE project, financially supported by CEA (Commissariat à l'Énergie Atomique), EDF (Électricité de France), IRSN (Institut de Radioprotection et de Sûreté Nucléaire) and AREVA-NP. The code solves, for each phase, Eulerian three-dimensional unsteady equations of mass, momentum and enthalpy, coupled through transfer terms between phases, and transport equation of a variable number of scalars. Parallel simulation efficiency of NEPTUNE_CFD has been tested on many platforms. Access to source code programs enable to modify existing models and also to test the build options to improve the performance of the code. Moreover, the excellent parallel performances of the code enable the implementation of multiphysics calculation of flows in actual flow configurations. In 2018, the main objective of the project is to continue the development a original n-Eulerian LES modeling approach which accounts for the subgrid particle segregation effect on the momentum transfer between the gas and the particles. Also, time will be dedicated to the development and validation of the modeling of heat and mass transfers, coupled with chemical reactions as to the numerical simulation of bioreactors.

Dernières publications:

- Neau H., Fede P., Ansart R., Simonin O., Renon N., Barbaresco P., Baudry C., Merigoux N., Massively Parallel Numerical Simulation of Hydrodynamics and Transfers in a Polydispersed Reactive Gas-Particle Fluidized Bed at Industrial Scale, Journées Calcul et Données JCAD'2018, 2018 -
- Yu, W.; Fede, P.; Climent, E. & Sanders, S. Multi-fluid approach for the numerical prediction of wall erosion in an elbow Powder Technology, 2019 , 354 , 561 - 583 - **doi:** pu.doi

SIMULATION DIRECTE ET MODELISATION DES ECOULEMENTS TRIDIMENSIONNELS TURBULENTS DE TYPE SILLAGE

Projet démarré en 2000

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Marianna Braza**

This project focuses on development of new simulation methods for the Direct Numerical Simulation as well as new strategies for turbulence modelling for unsteady flows around aerodynamic bodies, including deformable wing structures under the effect of electroactive morphing in order to increase the aerodynamic perfrmances. A new direction of this project focuses on the Fluid-Structure Interaction Modelling and Simulation. The project uses and develops advanced simulation tools for solving the Navier-Stokes equations in incompressible and compressible regimes, taking into account phenomena related to transition and turbulence. This project aims at investigating the successive stages of the flow transition towards turbulence around bodies. Concerning the high-Reynolds number regimes, this project aims at developing advanced turbulence modelling methodologies and Reduced Order Modelling (ROM) to accurately predict the aerodynamic coefficients in unsteady regimes, especially in the context of Fluid-Structure Interaction. Furthermore, the Electroactive Morphing concept of new generation of airvehicles is a major concern of the present project that aims at associating a very efficient Aeroelasticity integrated model, coupling the most advanced CFD to novel electroactive materials CSM (Computational Structural Mechanics), to achieve Morphing of aileron's structure. The CFD-CSM kernel is coupled with optimum shape design MDO, especially based to surrogate order modelling, to give the appropriate shape to the control surfaces in order to avoid nuisance phenomena (aileron flutter and vibration sources) and to improve manoeuvrability. This is achieved by acting on the Electroactive materials to enable deformation of the solid surface according to optimum shape design.

Dernières publications:

- 3. V. Shinde, E. Longatte, F. Baj, Y. Hoarau, M. Braza "Galerkin-free model reduction for fluid-structure interaction using proper orthogonal decomposition", in print, Journal of Computational Physics, 396, pp. 579-595, 2019 -
- S. Gsell, R. Bourguet, M. Braza, "One- versus two-degree-of-freedom vortex-induced vibrations of a circular cylinder at Re = 3900", Journal of Fluids and Structures, 85, pp. 165-180, 2019 - **doi:** pu.doi

4.2 Biomolécules, bioinformatique

Installation du logiciel MaxQuant pour l'analyse de données Proteomiques

Projet démarré en 2019

IPBS - Institut de Pharmacologie et de Biologie Structurale (UMR 5089)

Porteur de projet: **Emmanuelle Mouton**

Les logiciels d'analyses sont hébergés au sein de notre plate-forme sur des serveurs dédiés. Mais il arrive pour certains projets biologiques que ponctuellement nous ayons besoin de beaucoup de processeurs pour traiter des analyses volumineuses sur des calculs longs par exemple 80 fichiers (RAW data) de 2GB/fichiers répartis sur 24 processeurs logiques, nécessitent plusieurs jours d'analyses (jusqu'à 10 jours). Nous voudrions tester votre système associé aux temps de transfert des fichiers pour évaluer le gain de temps potentiel.

Etude des relations Structure-Dynamique-Fonction de dépolymerases d'intérêt pour la degradation du polyéthylène téréphthalate

Projet démarré en 2019

TBI - Toulouse Biotechnology Insitute

Porteur de projet: **Isabelle Andre**

De récents travaux ont révélé l'importance de résidus ainsi que d'éléments structuraux spécifiques à la surface de dépolymérases dans la modulation de leur activité de dégradation du polyéthylène téréphtalate (PET). S'inscrivant dans une démarche de développement de dépolymérases optimisées dans la dégradation du PET pour le bio recyclage du plastique, ce projet a pour objectif d'améliorer notre compréhension de l'impact de la dynamique de la structure de 8 PET dépolymérases connues sur leur activité de dégradation du PET. Nous analyserons plus particulièrement la dynamique du site de liaison du PET, afin de déterminer l'impact fonctionnel de la dynamique des résidus à la surface de ces enzymes sur l'interaction au PET. Dans ce contexte, nous souhaiterions effectuer des simulations de dynamique moléculaire de 500 ns de ces 8 PET dépolymérases dans 4 états distincts de leur cycle catalytique. Au total, nous voudrions donc réaliser 32 simulations de 500 ns. Conjointement aux simulations, des approches de design computationnel de protéines seront également mises en oeuvre pour guider l'ingénierie de ces dépolymérases en vue d'optimiser leur affinité vis-à-vis du PET. Afin de mener à bien ces travaux, nous souhaiterions obtenir un total de 700 000 heures CPU.

Transmission of Social Information

Projet démarré en 2019

EDB - Évolution et Diversité Biologique (UMR 5174)
Porteur de projet: **Alexis CHAINE**
Testing parameters for building social networks on bird data and how social information is transmitted across networks. The runs require bootstraps.

Dynamique d'interfaces complexes

Projet démarré en 2019

LGC - Laboratoire de Génie Chimique (UMR 5503)
Porteur de projet: **Micheline Abbas**
The aim of this project is to understand the effect of surface active molecules (amphiphiles, asphaletenes, ...) on the dynamics of liquid-liquid interfaces. The complex molecules modify the interfacial tension, induce a peculiar rheological behavior of the interface of visco-elastic nature, and influence the mass transfer between both phases. The presence of surface active molecules has a direct consequence on the response of the interface to external forcing, like breakup in turbulent flows. The objective of this project is to use numerical simulations, resolved at the meso-scale, in order to understand the dynamics of the interface.

Adsorption de polypeptides sur des surfaces métalliques - Une étude couplée ESI-MBD/STM/Modélisation

Projet démarré en 2019

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Nathalie Tarrat**
The study of the conformations and the self-assembly of biomolecules like polypeptides or polysaccharides on surfaces has emerged as a major topic in the research about molecules on surfaces (e.g. in the framework of biofilm adsorption on surfaces). However, the complexity of such molecules, together with the subtle interactions, both among them and between them and the surface, make it very difficult to systematically analyze their behavior on surfaces. To overcome these hurdles, we have decided to investigate relatively small systems as a first step. As an initial system, we have chosen the octapeptide "WWPPPPRR" on Au(111). This molecule is large enough to show already a flexible chain structure as we expect to find in extended

biomolecules, while still being small enough to be computationally accessible for global structure optimizations and local ab initio relaxations. By combining experiment (deposition with ESI-MBD and imaging with STM/AFM) and theoretical modelling, we aim at unravel the adsorption modes of polypeptides on metal surfaces.

Etude des voies d'introduction de deux espèces exotiques d'écrevisses envahissantes dans le réseau hydrographique de la Garonne

Projet démarré en 2019

EDB - Évolution et Diversité Biologique (UMR 5174)
Porteur de projet: **Géraldine Loot**
Biological invasions are one of the main drivers of the current biodiversity crisis, and the development of efficient measures for managing Invasive Alien Species (IAS) is needed. In complex environments such as freshwater ecosystems, the eradication of an IAS is nearly impossible once invasive species have successfully established. This suggests that IAS management actions should be engaged prior to their establishment to be efficient. Acting at early stages of biological invasions requires, however, having prior knowledge on the pathways used by IAS for colonizing a new environment, an information that is often lacking for many ecosystems. Here, we aim to determine the introduction pathways of two global IAS (the red swamp crayfish Procambarus clarkii and the spinycheek crayfish Faxonius limosus) in a meta-social-ecosystem composed by a network of artificial gravel pits. Specifically, we will use empirical genetic data (microsatellite markers), genetic data simulated under various competing colonization scenarios and approximate Bayesian computations coupled to random forest algorithms (ABC-RF) to (i) determine the most plausible invasion and colonization models for both species in the study area, and (ii) to infer from the best-fitting models values for key parameters related to the invasion process (e.g. numbers of introduced individuals, numbers of potential introduction sources and introduction dates). This study will allow us to draw recommendations for improving the management of IAS in complex environments aiming at preventing their initial introduction in novel ecosystems.

Analyse de données Single Cell RNAseq

Projet démarré en 2019

CRCT - CRCT UMR 1037 - Centre de Recherches en Cancérologie de Toulouse

Porteur de projet: **Frédéric PONT**

The Cancer Research Center of Toulouse (Centre de Recherches en Cancérologie de Toulouse, CRCT) has recently acquired the single cell RNA sequencing (scRNA-seq) technology. This technology measures the transcriptomes (gene expression profiling) of tens of thousands cells. Single cell transcriptomes allow the highest resolution of cellular states and functions of each individual cell in the context of its genuine microenvironment such as tumors and/or blood and normal tissues from human cancer patient. Since each scRNA-seq dataset represents a large amount of data to be explored by up-to-date algorithms developped at CRCT, it is thus crucial for our institute to access to the powerful computing resources of CALMIP.

Dernières publications:

- Single-Cell Signature Explorer for comprehensive visualization of single cell signatures across scRNA-seq datasets Frédéric Pont, Marie Tosolini, Jean J Fournié, Nucleic Acids Research, gkz601 - **doi:** pu.doi

Analyse de données Single Cell RNAseq

Projet démarré en 2019

CRCT - CRCT UMR 1037 - Centre de Recherches en Cancérologie de Toulouse

Porteur de projet: **Frédéric PONT**

Bonjour, Je fais partie du Pôle Technologique du Centre de Recherches en Cancérologie de Toulouse dirigé par F. Lopez. Ma collègue Marie Tosolini et moi même, nous nous occupons du traitement des données produites par l'ensemble du CRCT. Depuis 2017, nous faisons face à une demande croissante de traitement de données Single Cell RNAseq, particulièrement exigeant en calcul. Le Single Cell RNAseq (scRNAseq) est une nouvelle technique, publiée pour la première fois en 2009 {Tang2009}. Cette technique permet de mesurer le niveau d'expression des gênes sur une cellule unique. Les résultat sont donc beaucoup plus précis que les microarrays qui donnent l'expression des gênes d'un mélange. Il devient donc possible de découvrir de nouvelles populations de cellules et même d'étudier l'évolution des clones dans le temps {LaManno2018} ce qui est un enjeu majeur dans l'étude de l'évolution des tumeurs. Le scRNAseq fait la une des grands journaux {Svensson2018, Papalexi2018, Shalek2014}, et intéressera à court terme toutes les unités INSERM. Jusqu'à présent, nous effectuons la majorité des calculs sur un serveur bi Xeon E5-2687w-v3 - 128Go RAM. Les alignements de séquences sont effectués sur le cluster GénoToul qui possède déjà tous les logiciels nécessaire pour cette tâche. Cependant, certaines étapes du traitement des données ne sont pas adaptées à du calcul distribué sur cluster. Ce sont des applications multi-thread qui nécessitent beaucoup de RAM pour manipuler de grandes matrices de données (par exemple 23 000 lignes x 4 000 000 de colonnes) et notre serveur est de plus en plus à la peine. Je souhaiterais, au titre du pôle technologique du CRCT, demander l'ouverture d'un compte CALMIP pour l'année 2019 pour Marie Tosolini et moi même. Il m'est pour l'instant très difficile de fixer un nombre d'heures de calcul, puisque je dois effectuer des tests préalables afin de vérifier que les applications qui nous intéressent sont installables sur votre calculateur. Merci de prendre notre demande en considération. Bien cordialement F. Pont Références : F. Tang, C. Barbacioru, Y. Wang, E. Nordman, C. Lee, N. Xu, X. Wang, J. Bodeau, B. B. Tuch, A. Siddiqui, K. Lao, and M. A. Surani. mrna-seq whole-transcriptome analysis of a single cell. Nature methods, 6 :377–382, May 2009. G. La Manno, R. Soldatov, A. Zeisel, E. Braun, H. Hochgerner, V. Petukhov, K. Lidschreiber, M. E. Kastriti, P. Lönnerberg, A. Furlan, J. Fan, L. E. Borm, Z. Liu, D. van Bruggen, J. Guo, X. He, R. Barker, E. Sundström, G. Castelo-Branco, P. Cramer, I. Adameyko, S. Linnarsson, and P. V. Kharchenko. Rna velocity of single cells. Nature, 560 :494–498, Aug. 2018. V. Svensson, R. Vento-Tormo, and S. A. Teichmann. Exponential scaling of single-cell rna-seq in the past decade. Nature protocols, 13(4) :599, 2018. E. Papalexi and R. Satija. Single-cell rna sequencing to explore immune cell heterogeneity. Nature Reviews Immunology, 18(1) :35, 2018. A. K. Shalek, R. Satija, J. Shuga, J. J. Trombetta, D. Gennert, D. Lu, P. Chen, R. S. Gertner, J. T. Gaublomme, N. Yosef, et al. Single-cell rna-seq reveals dynamic paracrine control of cellular variation. Nature, 510(7505) :363, 2014. ========== Frederic PONT Centre de Recherches en Cancérologie de Toulouse, Bâtiment A, 1er étage Pôle Technologique du CRCT 2 avenue H. Curien, CS 53717, 31037 TOULOUSE Cedex1 - FRANCE - Email : frederic.pont@inserm.fr Tel : 33 5 82 74 15 97 (bureau) Tel : 33 5 82 74 15 92 (labo)

Exploring and applying GeoMetric Morphometrics imaging techniques to artistic iconographic record

Projet démarré en 2019

AMIS - Anthropologie moléculaire et Imagerie de Synthèse

Porteur de projet: **Ludovic ORLANDO**

The last decade has been home to massive technological innovations in the field of biomolecular archaeology and geometric morphometrics, which tremendously improved our capacity to reconstruct the living conditions and origins of past human societies. Even though the latter techniques are tailored to the analyses of body shapes and sizes, they have so far only been applied to the osseous archaeological record. Yet, their underlying design makes them readily applicable to the analysis of a whole range of forms that are found in different material and cultural sources, such as the artistic iconographic, figurine and statues record. In the last couple of years, my research laboratory has carried out preliminary work to obtain the proof-of-concept evidence that these technologies can retrieve reliable information about the shape, a number of production traits and coat-coloration patterns of past domesticate animals, especially the horse. The information gathered from historical paintings helped us identify the present-day breeds that most closely resemble the animals represented by artists, providing instrumental

information about the history of breed formation. Applied to older records, in particular pre-dating the invention of writing, these approaches hold the potential to provide quantitative information about the subsistence and farming economies of past societies. The next step of our project is aimed at diversifying the range of animals investigated, qualify the performance of the underlying methodology as a function of multiple confounding factors, and automate the acquisition of shape information from open-source image database, leveraging machine-learning techniques, in particular Conditional Random Field – Recurrent Neural Networks.

Exploration de la dynamique fonctionnelle et stratégies raisonnées d'ingénierie d'enzymes.

Projet démarré en 2019

TBI - Toulouse Biotechnology Insitute

Porteur de projet: **Sophie Barbe**

De plus en plus nombreux sont les travaux qui montrent que la flexibilité et les mouvements collectifs des (macro)molécules sont des composantes absolument essentielles des mécanismes d'interaction moléculaire et de l'activité catalytique des enzymes. Il en résulte que la vision statique de la catalyse enzymatique est insuffisante pour rendre compte du comportement cinétique de nombreuses enzymes. Dans le cadre de ce projet, l'un de nos objectifs est d'améliorer notre compréhension des liens étroits entre la structure, la dynamique et l'activité catalytique des enzymes. L'étude de ces liens nécessite l'exploration de différents types de mouvements (macro)moléculaires pouvant couvrir de larges échelles temporelles et spatiales. Nous ferons appel à des techniques de dynamique moléculaire pour explorer cette hiérarchie de mouvements. Les résultats de ces simulations seront confrontés à des données expérimentales acquises au sein de l'équipe (ou à travers des collaborations) et viseront ainsi à caractériser les facteurs structuraux et dynamiques impliqués dans l'activité, la spécificité et la sélectivité des protéines d'intérêt pour mieux comprendre différents processus biologiques. Sur la base de cette meilleure compréhension des relations structure-dynamique-activité des systèmes protéiques étudiés, nous identifierons des régions ad hoc à remodeler pour adapter et optimiser les protéines vis à vis de propriétés recherchées. Nous explorerons in silico la combinatoire de mutations sur ces régions à l'aide d'outils de design computationnel de protéines afin de proposer les séquences les plus pertinentes à tester au niveau expérimental. Nos travaux seront centrés sur l'étude de lipases et d'hémicellulases d'intérêt biotechnologique.

Cerberus, une plate-forme protéique pour la fonctionnalisation de la cellulose

Projet démarré en 2019

TBI - Toulouse Biotechnology Insitute

Porteur de projet: **Sophie Barbe**

Le projet Cerberus vise à créer une plateforme protéique permettant de fonctionnaliser à façon la cellulose. La cellulose est un polymère de glucose naturellement produit par les plantes et certaines bactéries. Très peu couteux, cette molécule est largement répandue dans l'industrie, son usage recouvrant les domaines de la papèterie, des matériaux, de la biotechnologie ou de la santé. Le projet Cerberus a été développé au cours du stage de Master 1 de dix étudiants de l'INSA de Toulouse et de l'Université Paul Sabatier, sous l'encadrement de chercheurs et d'enseignants-chercheurs du LISBP et du LBME. Le but étant de participer au concours iGEM (International Genetically Engineered Machine), concours international de biologie synthétique de renommé mondiale. La protéine plate-forme développée au cours du projet est composée de trois éléments. Une protéine centrale CBM3a permettant de reconnaitre la cellulose et de s'y associer, une streptavidine permettant de reconnaitre toute protéine biologique biotinylée et un acide aminé non naturel dont la fonction chimique permet de greffer toute molécule organique présentant une fonction alcyne. La streptavidine et l'acide aminé non naturel sont associés au CBM3a via des linkers composées de 42 à 32 acides aminés. Une partie du projet Cerberus a

consisté à modéliser la plateforme protéique. Pour cela, diverses méthodes de modélisation et de simulation moléculaires utilisant les structures cristallographiques des différentes protéines nous ont permis de réaliser et de valider un modèle en solution de la conformation des deux linkers. Cette partie du projet a fait appel aux ressources de calcul de CALMIP. Ces calculs ont nécessité 150 000 heures de temps de calcul (CPU) et généré 85 Go de données. L'ensemble des manipulations expérimentales et de modélisation a été présenté à Boston (USA), au cours de la finale de l'iGEM. Le projet Cerberus a remporté une médaille d'or, un prix et une nomination. Au vu de la qualité des données obtenues à l'issue du projet, les encadrants iGEM ont décidé de valoriser les résultats sous la forme d'une publication scientifique à comité de lecture. Pour cela, deux stages de master vont être financés afin de rendre publiables les données. Une partie de ces données concerne le modèle de la plateforme, pour lequel nous sollicitons de nouveaux les ressources du centre CALMIP. Nous estimons à 300000 heures nos besoins en temps de calcul afin de pouvoir réaliser les simulations nécessaires à la finalisation de cette étude.

Bilan de population multivariable pour la biologie

Projet démarré en 2019

TBI - Toulouse Biotechnology Insitute

Porteur de projet: **Jérôme Morchain**

The projet aims at developing multivariate population balance models for the numerical simulation of heterogeneous bioreactors. This objective requires a multiscale approach in which cellular behavior at the microscopic scale and large scale hydrodynamics at the reactor scale must be coupled. A multivariate population balance model approach was adopted to adress this question. Direct simulation based on Monte Carlo method was chosen to solve these equations. Beside the formulation of the problem and its numerical simulation, the project also aims at creating a database of numerical results that can be further used to assess the accuracy of Eulerian versions of the same population balance in view of their coupling with transport equation.

Etude de l'interaction de metallo-porphyrines avec des structures G-quadruplex d'acides nucléiques

Projet démarré en 2019

LCC - Laboratoire de Chimie de Coordination (UPR 8241)

Porteur de projet: **Jean-Luc Stigliani**

Guanine rich nucleic acids (DNA, RNA) may fold into three-dimensional, four-stranded arrangements referred to as G-quadruplex structures. Four guanines interact through Hoogsteen hydrogen bonds and form G-quartets that further undergo Pi-stacking interaction between each other creating a central ionic channel containing potassium ions. G-quadruplex structures are involved in fundamental processes of life (transcription, traduction, telomere maintenance etc). These peculiar structures, as relevant pharmacological targets, can be targeted by synthetic molecules. The presence of G-quadruplex structures in the genome of some viruses such as HIV-1, was recently evidenced. In the case of HIV-1 the G-quadruplex structures are located in crucial regions for the viral cycle. The team showed that G-quadruplex ligands based on metalloporphyrins inhibit HIV-1 infection in vitro with IC50 values similar to that of AZT, reference compound. Taking into account the structures of already active metalloporphyrins and with the help of modeling studies we will design and prepare highly specific ligands of viral G-quadruplexes that will then be tested in vitro and in vivo. Molecular modeling studies will consist of studying the effects of the central metal as well as the porphyrin's meso substituents on the interaction of the ligands with G-quadruplex, using molecular dynamics and hybrid quantum mechanics/molecular mechanics (QM/MM) methods.

Dernières publications:

- G-Quadruplex binding optimization by gold(iii) insertion into the center of a porphyrin. Dalton Transactions, 2019,48, 6091-6099 - **doi:** pu.doi

Investigating protein – ion-exchange chromatography surface interactions using Molecular Dynamics simulations

Projet démarré en 2019

TBI - Toulouse Biotechnology Insitute

Porteur de projet: **Jeremy Esque**

Ion-exchange chromatography (IEC) is a standard method for separation and purification of proteins. The protein adsorption is based on electrostatic interactions between the amino acid residues and the functional charged groups fixed on the chromatography surface. Experimentally, some physical parameters are calculated using the Steric Mass Action (SMA) model, such as the characteristic charge and the steric factor. These later are key to get a first insight of the binding mode of the protein during the chromatography process. However, there is still a lack of detailed information regarding molecular interactions involved in ion exchange chromatography. For these reasons, the aim of our project is first to compare experimental results (characteristic charge and steric factor) with those obtained through all-atomistic Molecular Dynamics (MD) simulations. MD simulations can help to better understand how the protein interacts with the chromatography support. α-chymotrypsin was chosen as a first protein model to validate our approach by comparing computational results with experimental data obtained in our lab. After validation of the procedure on this system, the next step will be to investigate a multi-constituent system, such as a mixture of α-chymotrypsin and lysozyme.

Dernières publications:

- Understanding adsorption behavior of α-chymotrypsin onto cation exchanger using all-atom molecular dynamics simulations - **doi:** pu.doi

Molecular modelling and design of catalytic scaffolds based on amyloid aggregates

Projet démarré en 2019

TBI - Toulouse Biotechnology Insitute

Porteur de projet: **Isabelle Andre**

Catalysis is widely accepted as one of the leading factors for promoting sustainable development. Although high selectivities have been achieved by tailored made catalysts, the synthesis of the latter is often obliterating the sustainability of the overall process. In this project, we aim at tackling this issue by developing hybrid catalysts made of a peptidic scaffold and a transition metal complex core (either by direct coordination, supramolecular interaction with a metal complex or though bioconjugation) to form a hybrid catalyst that can promote synthetically relevant catalytic events. A library of catalytic Amyloidogenic Peptides, varying in size and structures, will be designed and evaluated by a combination of in silico methods (computational protein design, molecular dynamics (MD) and replica exchange molecular dynamics (REMD) simulations) before being proposed for experimental testing via both chemical synthesis and protein engineering techniques. Overall, these sustainably produced hybrid catalysts are expected to open new dimension in fine chemical synthetic processes.

Dernières publications:

- Ben Imeddourene A., Esque J., André I.. 2018. Combining multi-scale modelling methods to decipher molecular motions of a Branching Sucrase from Glycoside-Hydrolase Family 70. Plos One 13(8):e0201323. (JCR=3.234) - **doi:** pu.doi

- Rovira C*., Alonso-Gil, Coines J., André I*. 2019 Conformational itinerary of sucrose during hydrolysis by retaining amylosucrase. Frontiers in Chemistry. - **doi:** pu.doi

High-resolution 3D structure determination of Pks13, the condensase of mycolic acids, by single-particle cryo-electron microscopy

Projet démarré en 2018

IPBS - Institut de Pharmacologie et de Biologie Structurale (UMR 5089)

Porteur de projet: **Cecile BON**

Type I polyketide synthases (PKS) are large multifunctional enzymes responsible for the biosynthesis of a structurally diverse range of natural products with a comparably broad spectrum of biological activities. The structure elucidation of PKS is of both fundamental and applied interest, with considerable potential for structure-based engineering and drug design. Most of the current knowledge about structure-function relationships of PKS has been deduced from structures of the related type I fatty acid synthase (FAS) enzymes and on combining high-resolution structural data for individual domains or didomains derived from PKS. Although there are not yet any atomic resolution structures of intact PKS, low-resolution models have been more recently derived from single-particle electron cryo-microscopy (SP cryo-EM) or by hybrid approach combining X-ray crystallography and small angle X-ray scattering (SAXS). Pks13 is a type I PKS involved in the final step of the biosynthesis pathway of mycolic acids, and is essential for the viability of mycobacteria. It has been the focus of intensive research aiming at characterizing its mechanism of action and druggability. In parallel with these studies, we have embarked on the structural characterization of such a complex megasynthase (186 kDa, 1733 residues comprising five catalytic domains interconnected by linker regions). Our strategy was to work on the full-length enzyme and on domains or fragments, and to use a combination of SAXS and crystallography to provide low- and high-resolution information, respectively. For instance, the crystal structure of a 52-kDa fragment containing the acyltransferase domain has been determined in different states. Our goal now is to make use of SP cryo-EM, which is nowadays "becoming a dominant technology", to determine the atomic structure of the full-length enzyme. Preliminary results, in collaboration with Célia Plisson-Chastaing (LBME, CBI) led to images of such quality that structure determination can now easily be foreseen. The objective of this application is to carry out single particle reconstruction from data already available and hopefully from data obtained at higher resolution on an even more powerful electron microscope. We would like to use RELION and Ctffind4, already installed on the CalMIP facilities, to be able to investigate the structure of Pks13 at the highest possible resolution, with the most time-efficient manner.

Modélisation de nanoparticules d'or et d'argent

Projet démarré en 2018

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Mathias Rapacioli**

In the present project, we investigate gold and silver clusters and nanoparticles. This topic is relevant from a fundamental side (understanding noble metal nanoclusters properties) but also in several contexts such as catalysis, health or sensors design. We are using the Density Functional based Tight Binding (DFTB) method, an approximated DFT scheme with a much lower computational cost than DFT, while conserving an explicit quantum description. We have developed a set of DFTB parameters and showed that they provide a good description of Ag/Au properties from clusters to bulk, opening the route to the modeling of large nanoparticles. The combination of this potential with global exploration schemes of the complex Au/Ag potential energy surfaces allows for the determination of structural and thermodynamical properties for systems containing from a few tens to hundreds

of atoms. More precisely, our current and future works consist in characterizing the structural nature of large gold clusters (regular or amorphous),establishing the size and charge effects on the heat capacity curves of Ag/Au clusters, as well as studying structural and thermodynamical modifications when clusters and nanoparticles are no longer in vacuum but deposited on a support.

Dernières publications:

- N. Tarrat, M. Rapacioli, J. Cuny, J. Morillo, J.-L. Heully, and F. Spiegelman. Global optimization of neutral and charged 20- and 55-atom silver and gold clusters at the dftb level. Computational and Theoretical Chemistry, 1107, 102 (2017) - **doi:** pu.doi **url:** pu.open_url
- L. F. L. Oliveira, N. Tarrat, J. Cuny, J. Morillo, D. Lemoine, F. Spiegelman, and M. Rapacioli. Benchmarking density functional based tight-binding for silver and gold materials: From small clusters to bulk. The Journal of Physical Chemistry A, 120, 42, 8469 (2016) - **doi:** pu.doi **url:** pu.open_url

Investigating Structure-Function Relationships of Carbohydrate-Active Enzymes to guide development of novel biocatalysts: A focus on Glycoside-Phospho

Projet démarré en 2018

TBI - Toulouse Biotechnology Insitute

Porteur de projet: **Jeremy Esque**

Oligosaccharides represent a class of very diverse biomolecules consisting in linear or ramified chains of sugar moieties or sugar derivatives that are linked together by different types of α or β osidic linkages. The wide structural diversity of oligosaccharides comes from both the combination of sugar moieties and the types of covalent linkages. These molecules are involved in a multitude of cellular processes, including cell signaling/differentiation, modulation of immune response, inflammation, and mediation of microbial and host-microbe interactions. Because of their highly versatile structures and biological functions, oligosaccharides are used for a broad range of applications in food (functional foods, prebiotics or as additives) and health (as drugs, drug carriers or vaccine intermediates) industries. Development of novel synthetic routes to access more easily to these complex carbohydrates is thus of utmost interest. Within this context, the current study will be integrated into a more ambitious project funded by the ANR, the project OLIGOMET (2016-2020), which aims at developing new bio-based synthetic routes for the efficient production of added-value oligosaccharides. Within this project, we will focus mostly on a particular family of Carbohydrate-Active enzymes (CAZymes), i.e. Glycoside Phosphorylases (GPs), among which several members have been recently discovered in our laboratory, the LISBP, using functional metagenomics (Tasse et al., Genome Res., 2010 ; Ladevèze et al., J. Biol. Chem. 2013 ; Cuskin et al., J. Biol. Chem. 2015). These enzymes, produced by gut bacteria, could play a role in polysaccharide phosphorolysis of plant cell wall and phosphorolysis of glycans from host intestinal epithelium. Nowadays, few studies have been dedicated to GPs. Therefore, better understanding their mechanism and their structure-function relationships seems to be crucial for developing their biotechnological applications. Our objective in fine is to use this fundamental knowledge to guide rational engineering of GPs toward novel catalytic reactions and substrates. These enzymes will be integrated in E. coli metabolic chassis to produce oligosaccharides of high-added value, mostly eukaryotic glycan cores and prebiotics.

Modélisation multi-échelle des molécules constitutives de la membrane des mycobactéries et leurs interactions avec la membrane de la cellule hôte

Projet démarré en 2017

IPBS - Institut de Pharmacologie et de Biologie Structurale (UMR 5089)

Porteur de projet: **Matthieu Chavent**

Mycobacterial infections, and in particular human tuberculosis (TB), remain major public health problems throughout the world, especially in developing countries. About two billion individuals worldwide are estimated to be carriers of Mycobacterium tuberculosis (Mtb), the etiological agent of human TB. This enormous reservoir of latently infected people, who may develop the disease decades after their infection and transmit the bacillus to other people, fuels the ongoing TB pandemic. We want to use molecular modeling to develop new strategies to understand the biological mechanisms of molecules involved in Mtb virulence and protection. Some of these molecules contribute to modulate the protective host immune responses. Using multi scale molecular dynamics simulations, we will study different types of molecules from complex lipids to proteins in order to shed lights on the biophysical mechanisms involving this molecules and also to develop a global understanding of the biological mechanisms taking place in the Mtb enveloppe.

Dernières publications:

- Interactions of the EphA2 Kinase Domain with PIPs in Membranes: Implications for Receptor Function - **doi:** pu.doi **url:** pu.open_url
- The conical shape of DIM lipids promotes Mycobacterium tuberculosis infection of macrophages - **doi:** pu.doi

Etudes par dynamique moléculaire d'hydrocarbures aromatiques polycycliques interstellaires et d'asphaltènes environnés

Projet démarré en 2017

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Aude Simon**

This project aims at characterizing polycyclic aromatic hydrocarbon (PAH) monomers and clusters in an environment using molecular dynamics simulations (MD). In these simulations, the electronic structure is computed on-the-fly using the self-consistent charge density functional based tight-binding approach. This project can be divided into two parts. We aim at characterizing: -(i)- (PAH)m(H2O)n clusters. This is an ongoing research project in our team, and it follows an ANR project which is ending (PARCS 2014-2017). Our goal is to characterize the structures, binding energies and vibrational and electronic spectra of PAH(H2O)n clusters in which the PAH is either planar or curved (typically pyrene and coranulene). This is done in collaboration with Nadia Ben Amor (LCPQ) and with experimentalists in Bordeaux (V. Blanchet and J. Mascetti). It is funded by the PCMI (physicochimie du milieu intertellaire) national program. This project has recently been extended to larger (PAH)m(H2O)n clusters and charged [(PAH)(H2O)]+ (collab. with C. Joblin's group, IRAP). -(ii)- asphaltenes in solution at the interface with liquid water. Asphaltenes are PAH derivatives that include heteroatoms and aliphatic chains. There exists varieties of asphaltenes that are present in fuel, coals, nanoparticles resulting from biomass combustion. Asphaltenes are regarded as the most enigmatic component in petroleum because of their negative influence on stabilizing the water-in-crude oil emulsion, that should be closely related to their self-aggregation. This has motivated experimental and theoretical studies (MD with force-fields) that sometimes lead to contradictory conclusions. In this context, we propose to characterize structural, energetic and dynamic properties of asphaltene molecules and clusters in solution at the interface with water, at the molecular level. We aim at determining asphaltenes' propensity to aggregate at the water interface, and with which orientation. The influence of the monomer size and chemical nature (presence of alkyle side chains, heteroatoms) on these properties will be studied. This new project in our group is done in collaboration with V. Pauchard (experimentalist, Engineering Department, City College of New York)and with the LGC (microfluidic experiments, ENSTA, Toulouse). It is now funded by the ANR project MUSCOFI.

Dernières publications:

- E. Michoulier, N. Ben Amor, Mathias Rapacioli, J. A. Noble, J. Mascetti, C. Toubin, A. Simon*, 'Theoretical determination of adsorption and ionisation energies of polycyclic aromatic hydrocarbons on water ice ', Phys. Chem. Chem. Phys. 2018, 20, 11941-11953 - **doi:** pu.doi
- A. Simon*, M. Rapacioli, E. Michoulier, L. Zheng, K. Korchagina, J. Cuny, Contribution of the Density-Functional based Tight-Binding Scheme to the Description of Water Clusters : Methods, Applications and Extension to Bulk Systems", Mol. Sim. "Water" Special Issue, 2019, 45, Issue 4-5 : "Water", 249-268 - **doi:** pu.doi

MoMA: Molecular motion algorithms for highly-flexible biomolecules

Projet démarré en 2016

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Juan Cortes**

Algorithms originating from robotics research have recently appeared as a complement or an alternative to classical methods to explore the conformational space of flexible bio-molecules. LAAS-CNRS is one of the pioneering labs in developing these novel approaches. These algorithms can be applied to small and middle-sized molecules (e.g. small peptides) using a single personal computer. However, analyzing large systems in reasonable computing time, while considering accurate models and full flexibility, requires parallelized implementations running on computer clusters. A few years ago we developed a distributed-memory implementation that we could successfully test on the MareNostrum supercomputer in Barcelona. We are now developing a more sophisticated parallelization strategy, combining shared memory and distributed memory operations, aiming at optimizing its performance using multi-core processors in current computer clusters. Preliminary tests in CALMIP (thanks to a "Test Project") have shown an excellent performance of this new implementation for proteins of different sizes. Our objective is to continue the development of these algorithms that will be applied to the study of intrinsically disordered proteins (IDPs) in the context of the PhD thesis of Alejandro Estaña, co-advised by Pau Bernadó (Centre de Biochimie Structurale, Montpellier).

Dernières publications:

- Alejandro Estaña, Nathalie Sibille, Elise Delaforge, Marc Vaisset, Juan Cortés, Pau Bernadó. Realistic ensemble models of intrinsically disordered proteins using a structure-encoding coil database. Structure, 27(2): 381-391.e2, 2019 - **doi:** pu.doi **url:** pu.open_url
- A Barozet, K Molloy, M Vaisset, T Simeon, J Cortés. A reinforcement-learning-based approach to enhance exhaustive protein loop sampling. Bioinformatics, 2019. - **doi:** pu.doi **url:** pu.open_url

Modélisation des interactions électrolyte/électrode dans les supercapacités de nouvelle génération

Projet démarré en 2015

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Alain Esteve**

This project proposes studying, by means of calculations at the atomic scale, the mechanisms of electrolytic species captured on the surface of active electrodes. Our study will aim to enable the realization and optimization of new generation of supercapacitors based on ruthenium / gold electrode, particularly in the synergistic development component between the electrolyte and the surface / subsurface of the electrode. The basic questions that will be addressed will be: identification and quantification of the electrolytic species in their mutual and net interaction in contact to the surface (retention times, potential chemical reactions, release of these

species). The calculations performed will be used to optimize the electrolyte in conjunction with that of the electrode surface.

Atlas Anatomique de Primates

Projet démarré en 2014

AMIS - Anthropologie moléculaire et Imagerie de Synthèse

Porteur de projet: **Jean Dumoncel**

The « Imagery » research team of the AMIS laboratory uses anatomical data essentially obtained by CT, micro-CT, or by synchrotron imaging. Through innovative technologies as well as academic and industrial collaborations (notably in the areas of image processing and the acquisition of high resolution data), we can better characterize the variability of phenotypic traits in teeth and bones amongst past and present populations of primates. Indeed, variability studies represent a prerequisite for future developments investigating evolutionary processes. Even if geometric morphometric studies (based on landmarks only) have proved to be useful, there is a need for automated tools and reproducibility anatomical comparison. Methods based on deformable models are increasingly used in medicine and should be better implemented in biological investigations as ours. We use a program developed by Stanley Durrleman (INRIA Researcher, ICM, Brain and Spine Institute). It computes anatomical atlases based on deformation maps without landmarks. These statistical atlases are based on average templates and local deformations, and then used to classify anatomical data.

Dernières publications:

- J. Dumoncel, J. Braga, E. Courcelle, N. Renon. Comparaison de structures anatomiques et calculs intensifs en paléoanthropologie. In: Journées Calcul Données (JCAD), 2019, Toulouse, présentation podium -
- A. Urciuoli, C. Zanolli, D. Begun, S. Almécija, J. Dumoncel, S. Moyà-Solà and D. M. Alba. A deformation-based geometric morphometric analysis of the vestibular apparatus in the Miocene apes Hispanopithecus laietanus and Rudapithecus hungaricus. In: 88th Annual Meeting of the American Association of Physical Anthropologists (AAPA), 2019, Cleveland, présentation podium. -

Cartographie et étude des duplications segmentaires intra- et interchromosomiques

Projet démarré en 2014

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)

Porteur de projet: **Sylvain Cussat-blanc**

Segmental duplications (SDs) are DNA sequences of minimum 1kb and 95% identity between copies. They represent a key substrate for gene conversion, and an underestimated source of genomic diversity. However, few algorithm have been designed to extract efficiently SDs from complex genomes. In 2016, we have developed ASAGRT, a powerful algorithm searching for SDs in any genome properly assembled. We have compared ASGART performances in regard to the most similar algorithm existing in literature. Comparative performances performed on 5 model organisms showed that ASGART is systematically better than Last and than Mummer (in CPY time and memory used). However, if SD mapping is easy and fast at the intra-chromosomic level, it appears more complicated at inter-chromosomic level (ull genome). We now, need to go futher on SD's full genome acquisition, probably by modify ASGART and the alignment procedure. Once solved we will be able to address 2 fundamental biological questions: 1) the role played by SD on sex chromosomes as an alternative substrate for gene conversion and 2) the real duplicative scenario that affected the vertebrate genomes (exploring fish genomes).

Etude structurale de particules pré-ribosomiques eucaryotes par cryo-MET et analyse d'images

Projet démarré en 2014

LBME - Laboratoire de Biologie Moléculaire eucaryote (UMR 5099)

Porteur de projet: **Célia Plisson-Chastang**

Ribosomes are ubiquitous macromolecular machines ensuring the translation of mRNA into proteins. The synthesis of ribosomes is one of the major cellular activities, both from a quantitative and a qualitative point of view. Ribosomes are composed of a small and a large subunits, respectively termed 40S and 60S in eukaryotes. Assembly of those huge ribonucleoprotein complexes is a very complex and dynamic process, that requires more than 200 maturation factors interacting transiently with the forming particles. Ribosome biogenesis defects have recently been associated to an increasing list of human genetic diseases and cancers; understanding those diseases calls for a better knowledge of ribosome maturation pathways in human cells. Our group focuses on studying the mechanisms enabling the assembly of eukaryotic ribosomes, using both yeast and mammal cells as models. To do so, we notably use cryo-electron microscopy coupled to image analysis techniques to determine the 3D structures of pre-40S particles. Cryo-electron microscopy (cryo-EM) is a very powerful method that allows determination of the 3D structure of very large complexes. We have already made use of cryo-EM and image analysis on the computing facilities of CalMIP to solve the first 3D structure of a pre-40S particle purified from human cells, to 19 Å resolution. This work has given rise to a first scientific article, published in the journal Nucleic Acids Research. We have more recently acquired cryo-EM datasets of other pre-40S particles purified at various maturation steps, either from baker's yeast or human cells, that we have processed using CalMIP's computational facilities. The various 3D reconstructions that we have obtained, at ~3-4 Å resolution allow us to propose the first morphogenesis depiction of the assembly of the eukaryotic small ribosomal subunit. Based on these excellent results, we would like to use CALMIP to study the 3D structure of other precursors to the small tibosomal subunit.

Dernières publications:

- Structure of a human pre-40S particle points to a role for RACK1 in the final steps of 18S rRNA processing Natacha Larburu; Christian Montellese; Marie-Francoise O'Donohue; Ulrike Kutay; Pierre-Emmanuel Gleizes; Celia Plisson-Chastang Nucleic Acids Research 2016 - **doi:** pu.doi **url:** pu.open_url
- Conformational proofreading of distant 40S ribosomal subunit maturation events by a long-range communication mechanism; Valentin Mitterer, Ramtin Shayan, Sébastien Ferreira-Cerca, Guillaume Murat, Tanja Enne, Dana Rinaldi, Sarah Weigl, Hajrija Omanic, Pierre-Emmanuel Gleizes, Dieter Kressler, Celia Plisson-Chastang and Brigitte Pertschy - **doi:** pu.doi **url:** pu.open_url

Développement et validation de méthodes pour la conception assistée par ordinateur de protéines

Projet démarré en 2013

TBI - Toulouse Biotechnology Insitute

Porteur de projet: **Sophie Barbe**

Ce projet porte sur le développement et la validation de nouvelles méthodes et outils de design computationnel de protéines (Computational Protein Design, CPD). Au cours de l'année 2019, nous allons poursuivre les développements visant à étendre nos méthodologies à la résolution de problèmes de design multi-états et multi-objectifs ainsi qu'à combiner et intégrer dans le processus de design de la connaissance extraite par apprentissage automatique de la biodiversité des séquences de protéines. Fondées sur une association de techniques algorithmiques développées en intelligence artificielle et en biologie structurale computationnelle, ces nouvelles méthodes devraient permettre de fournir des solutions uniques ou de petites librairies de mutants qui puissent être plus facilement et rapidement criblées au niveau expérimental tout en augmentant les chances de construire

les protéines dotées des propriétés ciblées. Les méthodes développées seront validées sur un grand nombre de systèmes protéiques représentatifs de différents problèmes de design des protéines.

Dernières publications:

- Simoncini D, Zhang KYJ, Schiex T, Barbe S. (2018) A Structural Homology Approach for Computational Protein Design with Flexible Backbone. Bioinformatics. In press -
- Charpentier, A., Mignon, D., , S., Cortés, J., Schiex, T., Simonson, T., Allouche, D. (2018) Variable Neighborhood Search with CostFunction Networks to Solve Large Computational Protein Design Problems. Journal of Chemical Information and Modeling. In press -

Simulation à l'échelle atomique pour l'oncologie structurale

Projet démarré en 2012

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Marie Brut**

This request supports a long-term collaboration with CRCT-INSERM and aims at proposing new strategies to target Ras oncoproteins, mutated in ~30% of all human tumors. Our team has a strong background in the treatment of biological issues, notably with enzymes as therapeutic targets. Our collaboration with CRCT to investigate some mechanisms involved in the regulation activity of Ras family proteins lead us to identify new mutations allowing to modulate NRas activity, mutations that we need to characterize on both structural and chemical sides. To this end, we use both traditional tools from molecular simulation (DFT and Molecular Mechanics) and "lab-made" tools that allow original in silico experiments on biomolecules. We complement this strategy thanks to steered QM/MM calculations to understand the local chemistry induced by the mutations we have predicted. Our ultimate goal is to propose a new therapeutic strategy able to mimic the effect of such mutations. After years of work on NRas, this strategy is validated and proved its ability to restore NRas activity through the prediction of new mutations. Such mutations have been validated after being tested in vitro and in cellulo, which lead us to establish new collaborations with pharmacologists in order to find a drug able to mimic their effect. This work is actually ongoing, supported by the Occitanie Region and the "SATT". Now, we aim at applying the same simulation protocol to another target: Kras. Along the same line, and through new collaboration, we also expand the list of target to explore, with a new focus on the protein cGas for cancer immunotherapy. This enzyme, recently discovered, participates in the early steps of a pathway responsible for the innate immune system of the cell, after being activated by circulating DNA. The chemical reactions occurring in its active site, as well as DNA activation, are poorly understood, but crucial to target cGAS. We recently started to work on this protein, mainly through QM/MM simulations to elucidate its structure/activity mechanisms.

Dernières publications:

- Tichauer et al. Water distribution within wild type N-ras protein and its oncogenic mutations at position 61 during unrestrained QM/MM molecular dynamics. Biophysical Journal 115 (2019), 1417-1430 - **doi:** pu.doi **url:** pu.open_url
- Tichauer et al. Hybrid QM/MM vs pure MM molecular dynamics for evaluating water distribution within p21Nras and the resulting GTP electronic density. J Phys Chem B 123 (2019), 3935-3944 - **doi:** pu.doi **url:** pu.open_url

Modélisation de complexes de métaux de transition. Optimisation de géométrie et structure électronique.

Projet démarré en 2012

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Jacques Bonvoisin**

The project concerns the modelization of metallic complexes. In this project we would like to follow the electronic properties of these complexes. Modelization means geometry optimization as well as prediction of electronic properties. We would like to predict the IR and UV-Vis spectrum. The different forms of this complexes will be studied by DFT in order to have a good understanding of the electronic and magnetic properties by using the resident GAUSSIAN program on CALMIP. We may also vary the ligands around the metallic atom in order to see the impact on the electronic properties and the UV-Vis spectrum. I would like to use the CALMIP platform because the system under study cannot be modelized with our resource; the computed time would be too long.

Dernières publications:

- "Spectral signature of a Ru(II, III, IV) complex: a combined experimental and theoretical investigation" J. Bonvoisin & I. Ciofini. Dalton Transactions (2013) 42, 7943-7951. - **doi:** pu.doi
- "Two-Dimensional Halogen-Bonded Self-Assembly of copper beta-diketonato Complexes" Fabien Silly, Christine Viala & Jacques Bonvoisin. J. Phys. Chem. C (2018) 122, 17143-17148 - **doi:** pu.doi

Spectroscopie in silico de systèmes biologiques et de phases liquides. Apport de la dynamique moléculaire classique et ab-initio.

Projet démarré en 2007

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Franck Jolibois**

Understanding the structural, dynamic and spectroscopic properties of chemical systems in the liquid phase at different temperatures and / or at different pressures is a matter of fundamental importance both in biological, physical or chemical sciences. As part of the theoretical simulation of such systems , the accurate modeling of the interactions and a correct sampling of the configuration space is a prerequisite for calculating spectroscopic parameter . We propose to conduct ab initio molecular dynamics studies on three liquid systems with a priori different properties: water (H2O) , ammonia (NH3) and nitromethane (CH3NO2). A DFT approach within periodic boundary conditions and using plane wave basis sets will be used for calculating the energy and gradients . The validation of our results will be performed by comparing two types of parameters to existing experimental data: the structure of the liquid obtained by calculating the radial distribution function and a spectroscopic signature with the theoretical determination of NMR chemical shielding. We intend, through this project, to establish a comprehensive and effective strategy for the precise modeling of liquid systems. For this, different parameters will be analyzed on the three aforesaid chemical systems : the inclusion of dispersion forces and exact exchange in DFT functional, the necessity to introduce nuclear quantum effects , the number of molecules explicitly used in the primitive box for the calculation of the energy, gradients and NMR parameters, the influence of isotope effects on the hydrogen atom and the influence of temperature. In parallel with this study, we also propose to exploite the capability of classical molecular dynamics to explore configurations space of large systems in order to investigate the structural properties of "bio-inspired" molecules (peptoids). These studies coupled with the calculations of specific spectrocopic properties (mainly NMR and Circular Dichroïsm) and their comparison to experimental spectra will allow the elucidation of their 3D structures.

Dernières publications:

- Exploring the Conformation of Mixed Cis–Trans α,β-Oligopeptoids: A Joint Experimental and Computational Study. G.Dumonteil, N.Bhattacharjee, G.Angelici, O.Roy, S.Faure, L.Jouffret, F.Jolibois, L Perrin, and C.Taillefumier, J.Org.Chem. (2018) 83, 6382–6396. -
- Evaluation of Gas to Liquid 17O and 1H Shift of Water: a Test Case for Molecular and Periodic Approaches. J.Cuny, F.Jolibois and I.C.Gerber J.Chem.Theo.Comp. (2018) 14, 4041–4051 -

Etude des propriétés structurales, spectroscopiques et dynamiques de Molécules et Agrégats

Projet démarré en 2000

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Fernand Spiegelman**

This project is a long-term project on the structural, spectroscopic, dynamical and thermodynamical properties of various complexes and clusters (molecular complexes, homogeneous clusters, atoms and molecules adsorbed or embedded on/in clusters). The methodology is based on the development of the Density Functional Tight Binding method for a quantum description of the electronic structure and the combination with various simulation codes for on-the-fly classical or quantum molecular dynamics to derive structural and spectroscopic properties. The advantages of DFTB are: (i) DFTB efficiency evolution towards very large systems, (ii) combination with dynamics and global exploration methods to derive finite temperature properties, (iii) combination with Path-Integral Molecular dynamics. The current applications are: (i) structure, reactivity and thermodynamics of water clusters containing impurities for atmospheric chemistry, (ii) structure, spectroscopy (IR and electronic) and fragmentation dynamics of carbonaceaous complexes and PAH clusters (poly-aromatic hydrocarbons) displaying astrochemical interest.

Dernières publications:

- Christine Joblin, Gabi Wenzel, Sarah Rodriguez Castillo, Aude Simon, Hassan Sabbah, et al., Photo-processing of astro-PAHs. Journal of Physics: Conference Series, IOP Publishing, In press - **url:** pu.open_url
- Luiz F. L. Oliveira, Nathalie Tarrat, Jérôme Cuny, Joseph Morillo, Didier Lemoine, Fernand Spiegelman, Mathias Rapacioli,, Benchmarking Density Functional Based Tight-Binding for Silver and Gold Materials: From Small Clusters to Bulk, J. Phys. Chem. A 2016, 120, 42, 8469-8483. - **doi:** pu.doi

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4.3 Sciences de l'Univers et de la Terre

Installation et tests du modèle de chimie transport GEOS-Chem

Projet démarré en 2019

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Bastien Sauvage**

J'utilise actuellement le modèle d'atmosphère 3D chimie transport GEOS-Chem, développé par l'Université d'Harvard, sur le cluster du laboratoire d'Aérologie, modèle pour lequel nous faisons aussi des développements et qui nous sert dans notre domaine de recherche. Dans le cadre d'une nouvelle thèse, nous souhaiterions effectuer des simulations sur l'ensemble du globe et sur 20 années, avec des sorties mensuelles et une résolution horizontale de 0.5x0.6° (simulation de base), ainsi que plusieurs tests de sensibilité (aux émissions, à la météorologie,etc...) sur la même durée, fréquence et configuration Le cluster nuwa ne nous permet pas de traiter des simulations si longues puisqu'il faudrait par exemple 150 jours pour la simulation de base, en version openmp (sur 1 noeud à 16 coeurs) Nous souhaiterions donc dans un premier temps tester le modèle en openmp mais aussi en mpi sur CALMIP, pour évaluer la configuration la plus adaptée en fonction de la technologie et des noeuds CALMIP. En espérant que cela soit concluant, nous souhaiterions dans un second temps demander des heures de calculs et du stockage, pour l'ensemble des simulations à effectuer

Inversion de formes d'onde altimétriques

Projet démarré en 2019

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Fernando NIÑO**

Depuis juillet 2018 nous avons mis en place au laboratoire un outil d'inversion de formes d'ondes altimétriques : en utilisant les données radar des satellites altimétriques et un simulateur de ces données, nous sommes en mesure de constituer de bases de données de "formes d'onde" altimétriques (les echos radar) à partir desquelles nous appliquons des techniques d'apprentissage automatique avec des réseaux profonds. La méthodologie prévoit deux phases distinctes: la génération de données simulées à partir de notre code de simulation (du python avec un noyau de calcul en C), puis l'intégration de ces données dans le réseau de neurones en tant que base d'apprentissage. Aujourd'hui les performances du réseau sont très bonnes si l'on s'intéresse aux données altimétriques en hydrologie, autour des grands fleuves (e.g. Amazone) mais un peu moins bien dans le domaine côtier, plus complexe. Nous avons besoin d'augmenter le nombre de données dans la base d'apprentissage, et créer un nouveau réseau de neurones avec ces nouvelles données. Aujourd'hui nous utilisons essentiellement un PC linux équipé d'un GPU GTX 1080, mais il est insuffisant pour le type d'application envisagé. On a déjà utilisé le cluster du CNES, avec des bons résultats, mais il n'a encore que 4 GPUs, et la demande est telle qu'ils sont déjà complètement saturés. Ce projet de test vise donc à déployer sur Calmip toute l'infrastructure logicielle de simulation et apprentissage profond, pour établir si l'utilisation de cette méthodologie peut s'améliorer dans le domaine côtier, et produire quelques résultats qui visent à indiquer quelle précision peut être atteinte. Le couplage avec des modèles océaniques haute résolution, comme Symphonie qui tourne déjà à Calmip, est intéressant et déjà envisagé.

Tropical Atlantic Climate Variability

Projet démarré en 2019

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Serena Illig**

Project 19002 is a high-resolution regional modeling project for the study of the interannual mode of variability in the equatorial and southeastern Atlantic Ocean. The Atlantic zonal mode of variability is associated with sea surface temperature anomalies near the equator, peaking in the Gulf of Guinea. Warm events are named Atlantic Niños because their dynamics resemble the equatorial Pacific El Niño mode. Along the coasts of Angola and Namibia, extreme warm interannual events - the Benguela Niños - occur every few years and affect the regional climate, the fish habitats, and the ocean productivity. Atlantic Niños peak in boreal summer (Jun-Jul), while Benguela Niños occur preferentially in Austral Autumn (Mar-Apr). Our objective is to highlight the link between these two modes of variability that are both associated with the propagation of eastward-propagating equatorial and coastal waves, forced in the western/central equatorial basin by surface zonal wind modulation (Figure 1). We want to elucidate why the Benguela Niño events occur 1 month prior to the warming in the eastern equatorial basin, which is counterintuitive with regards to their forcing mechanism. This project takes advantage of developments in ocean modeling (hydrodynamic, biogeochemical and atmospheric) carried out by the PI within CALMIP P1044 and P1134 projects. It is based on the use of the ROMS/CROCO community ocean model. Our need for the first semester of 2019 is estimated to 200000h and will be dedicated to the development of an interannual Tropical Atlantic ROMS regional configuration and its validation against available observations. We will then perform composite of sensitivity experiments to the season at which equatorial waves propagate, in order to quantify the importance of the seasonal variations of the equatorial and coastal ocean stratification in controlling the thermodymical response to the wave propagations.

Mesoscale air-sea interactions in the western Tropical Atlantic

Projet démarré en 2019

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Julien Jouanno**

Recent studies have shown the importance of mesoscale air-sea interactions in determining the ocean dynamics. In particular, it has been shown that mesoscale Thermal Feedback (TFB) and Current FeedBack (CFB) partly control the Western Boundary Currents dynamics and that the CFB also induces a sink of energy from mesoscale eddies to the atmosphere, causing a large dampening of the mesoscale activity and a subsequent reduction of the eddy-mean flow interaction (i.e., a reduction of the inverse cascade of energy). Nonetheless, the Wave FeedBack (WFB) impacts on the atmosphere and the ocean are generally ignored although they could have a significant effect on e.g., the energy exchange between the ocean and the atmosphere, and, thus, the TFB, CFB, and the ocean dynamic. The western Tropical Atlantic (which we define as the region between 80W-30W and 5S-20N) is particularly well suited to unify our understanding of the mesoscale air-sea interactions in tropical areas, and to specifically tackle the question of the role of varying upper ocean stratification in determining the wind response : i) early results suggest that the so-called TFB and CFB of the mesoscale eddies on the atmosphere are particularly active in this region and may contribute to shape the eddy properties and regional mean state (see Figure 1), ii) it gathers a broad range of upper ocean conditions influenced by the world largest river runoffs (Amazon and Orinoco river plume, see Figure 2) and tropical cyclone activity, and iii) the region will hold the EUREC4A intensive atmospheric field campaign in January-February 2020 (http://eurec4a.eu) and possibly intensive oceanic field campaigns (project EUREC4A-OA) both dedicated to air-sea coupling.

Intermittence multi-échelle de champs océaniques

Projet démarré en 2019

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Joël Sudre**

This new request is to perform a comparative study between high-resolution regional modeling and satellite data for characterizing the turbulent flows in different areas of the world ocean (Bay of Biscay, Upwelling of Peru/Chile and Gulf of Mexico). Model experimentation will be carried out both in idealized conditions (Gulf of Mexico) and in more realistic conditions. The three areas are selected for their contrasted meso-and submesoscale activities. A comparative approach with new methodologies originating from the study of turbulent systems (singularity and intermittence exponents) will not only transpose tools and study methods into different ecosystems but it will also allow an improved understanding of the specificities of each system in relation to fine scale processes that control the ocean mean state and ecosystem conditions. This project takes advantage of developments in coupled modeling (hydrodynamic, biogeochemical and atmospheric) carried out by the SYSCO2 team (LEGOS) within CALMIP P17016 (PI. S. ILLIG ends end of 2018) and P1044 (PI. B. Dewitte) projects. It is based on the use of three community models: the ROMS-CROCO hydrodynamic model, the WRF atmospheric model and the BioEBUS biogeochemical model. Our need for the first semester of 2019 is estimated to be an amount of 250 000h, and will concern the development of two complementary sub-projects dedicated to the study of turbulent flows in the upwelling system of Peru/Chile and in the Gulf of Mexico.

Structure et variabilité du champ magnétique stellaire: impact sur l'évolution des planètes proches de leur étoile

Projet démarré en 2019

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Laurène Jouve**

This project aims at modeling the magnetic field of low-mass stars (less than 1 solar mass) at different stages of their evolution : from the young stages when the star is still surrounded by a protoplanetary disk where planets form to later stages where the star possesses an assembly of planets. At all these stages, the convective envelopes of these stars are know to be the seat of dynamo action, a process through which the plasma motions twist and shear the magnetic field lines to amplify and maintain magnetic energy against Ohmic dissipation. Recent observational and numerical works show that the characteristics of the stellar magnetic field strongly vary with the internal structure of the star (i.e. the size of the convection zone) and the rotation rate. The large-scale structure and the variability of these stellar magnetic fields are likely to deeply modify the interaction between the star and the protoplanetary disk during the early phases of the star evolution. In particular, the stellar magnetic field generates a cavity between the surface of the star and the inner edge of the disk, called the magnetospheric gap. This magnetospheric gap thus truncates the disk at a certain distance from the star, depending on the stellar magnetic field structure and amplitude. While they form, planets have the tendency to get closer to their star through gravitational interactions with the disk. If the disk is truncated, the migration stops. We wish in this project to better understand how the stellar magnetic field structure and variability may impact the history of planet migration by modeling both the internal dynamo processes at the origin of the stellar fields and the dynamics of protoplanetary disks and of planets migrating inside them. The project is thus divided into two main steps, for which a PhD student and a postdoctoral fellow with experience in numerical modeling have just joined the IRAP laboratory.

Modélisation de la qualité de l'air en aéroport

Projet démarré en 2019

ONERA - Office National d'Etudes et de Recherches Aéronautiques

Porteur de projet: **Claire Sarrat**

In this study, a new approach to study the impact of air traffic on air quality is proposed. The pollutants concentrations are calculated at 10 m resolution using a Large Eddy Simulation (LES) model in order to identify the most affected areas of an airport platform. A day of air traffic is simulated using ensemble forecasting meteorological simulations for initialization and lateral boundaries conditions. In order to estimate the aircraft emissions the Air Transport Systems Evaluation Infrastructure (IESTA) is used. IESTA is coupled with the non-hydrostatic meso-scale atmospheric model Meso-NH using LES (Large Eddy Simulation) capabilities. The detailed cartography of the airport distinguishes between grassland, parking and terminals, allowing to compute exchanges of heat, water and momentum between the different types of surfaces and the atmosphere as well as the interactions with the buildings using a drag force. The dynamic parameters like wind, temperature, turbulent kinetic energy and pollutants concentrations are computed at 10 m resolution over the 9 x 9 km airport domain. The reactive chemistry is taken into account for gaseous compounds while particulate matter (PM10 or PM2.5) are considered as passive tracers. An ensemble of simulations is computed in order to estimate the variations due to large scale conditions.

Structure d'atténuation de Mars à partir des données InSight/SEIS

Projet démarré en 2019

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Ludovic Margerin**

The objective of this proposal is to take advantage of recent developments in the fields of random and scattered seismic waves and experimental mineralogy to develop original seismological and physical models of Mars interior

based on the analysis of the data that will be collected by the SEIS instrument in the framework of the InSight mission to Mars. Thanks to his selection as Participating Scientist by CNES, the applicant (L. Margerin) will have direct access to the SEIS data. We request 150000 CPU hours to perform numerical modeling of the diffuse field. Based on the modeling of the high-frequency wavefield with the aid of multiple-scattering radiative transport models, we will derive global attenuation profiles for the Interior of Mars. By separating the contributions of scattering and absorption to the total seismic attenuation, we may able to detect the presence of volatiles in the crust. Our modeling approach is based on the elastic transport equations that will be solved in spherical geometry using a Monte-Carlo approach combining ray-tracing and the accurate simulation of mode coupling and scattering anisotropy at each scattering events. The code is written in the C language, employs routines of the GSL for the selection of random numbers as well as the Message Passing Interface for parallelization. On a single processor, a typical run is of the order of 50 hours or more depending on the desired spatio-temporal resolution. As the Interior of Mars is still poorly determined, a sufficiently large number of runs are required. Hence, in a first step, we request 150000 hours corresponding roughly to 3000 numerical experiments.

Modélisation sismique des étoiles sous-géantes

Projet démarré en 2019

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Sébastien Deheuvels**

L'astérosismologie (étude des oscillations des étoiles) est le seul outil qui permette actuellement de sonder les intérieurs stellaires. Le développement de missions spatiales en partie dédiées à l'astérosismologie (CoRoT, Kepler, TESS, bientôt PLATO) a ouvert un âge d'or pour la discipline et a déjà permis de revisiter de nombreuses questions ouvertes en physique stellaire. La sismologie des sous-géantes présente un intérêt tout particulier. Les étoiles atteignent ce stade lorsque leurs réserves en hydrogène au coeur sont épuisées. Alors, leur coeur se contracte et leur enveloppe se dilate (d'où le nom de "sous-géantes"). D'un point de vue sismique, elles présentent le grand intérêt d'osciller suivant des modes dits "mixtes", qui se comportent à la fois comme des modes de pression dans l'enveloppe et comme des modes de gravité dans le coeur. La sismologie de ces étoiles permet grâce à ces modes de sonder le coeur stellaire, qui est généralement inaccessible. Notre projet consiste à exploiter ces étoiles pour progresser dans une des principales questions ouvertes actuelles en physique stellaire, celle de la taille des coeurs convectifs. Pour les étoiles qui possèdent un coeur convectif, connaître précisément la taille de ce coeur est crucial car il joue le rôle de réservoir pour les réactions nucléaires. Or, on sait qu'un certain nombre de processus physiques encore méconnus (comme l'overshooting) viennent étendre les coeurs convectifs. Cela représente une des principales sources d'incertitudes actuelles sur l'âge des étoiles. Nous avons déjà montré que l'utilisation des modes mixtes permet de mesurer la taille des coeurs convectifs et nous avons développé une méthode de modélisation sismique pour cela (Deheuvels & Michel 2011). Nous souhaitons désormais appliquer cette méthode aux sous-géantes observées par le satellite Kepler. Cela nécessite le calcul de nombreux modèles d'évolution stellaire en parallèle, ce qui justifie notre besoin de ressources à CALMIP.

Profil d'atténuation dans la Lune

Projet démarré en 2019

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Marie Calvet**

Recent developments in lunar studies show that the surface layer of the Moon might present substantial porosity down to greater depths than previously expected. These superficial heterogeneities strongly affect the seismic signal. Our main purpose is to find the diffusivity and the absorption profiles within the Moon, two key parameters

to describe the heterogeneity of the Moon. To describe the propagation of seismic energy within the Moon, we solve the diffusion equation in 3D axisymmetric geometry. Synthetic seismic energy envelopes will be next compared to Apollo seismic records. We plan to implement a bayesian approach to explore the space of parameters. We hope to propose a new heterogeneity model of the Moon that will give new constraints on its evolution.

Dernières publications:

- K. Gillet, L. Margerin, M. Calvet, M. Monnereau, Scattering attenuation profile of the moon : implications for shallow moonquakes and the structure of the megaregolith, Phys. Earth Planet. Int., 262, 28-42, 2017. - **doi:** pu.doi

Effets semi directs et indirects des aérosols sur le régime de précipitation à l'échelle du massif pyrénéen

Projet démarré en 2019

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Véronique Pont**

The Pyrenean massif atmosphere is largely influenced by both anthropogenic and natural sources of aerosols. Indeed, under the various possible meteorological influences, Saharan dust, marine aerosols, biomass burning aerosols, aged carbonaceous aerosols as well as fresh ones, and the associated non organic ones can be melt in the Pyrenean atmosphere. Through a regional modeling exercise compared to numerous available datasets over this area, we tend to estimate the impact of such aerosol content on the precipitation over this massif. The approach is as following: • Regional modeling exercise is conducted with the Regional Climate Model REGCM4, running with ECMWF meteorological fields and ECCAD and GFAS emission inventories for gases and aerosols from anthropogenic and field fires sources from January 2010 to December 2020 • Optical aerosols properties are evaluated thanks to the Pic du Midi aerosol properties database from the ACTRIS network. Wind fields and thermodynamic parameters are evaluated with the reanalysis ECMWF products. Aerosol atmospheric content is also compared to MODIS AOT database. • Next step consist in estimating the direct and indirect radiative forcings of this atmospheric aerosol content over the Pyrenees by making the difference between simulations with and without carbonaceous aerosols • The semi direct and indirect effects are thus quantified through the evaluation of the temporal and spatial variability of precipitations (comparing with TRMM and CRU precipitations fields) over the matching period This approach is thus prospective for the years when precipitation data are not available, and enable to understand how the atmospheric aerosol composition over the Pyrenees can force the signal in precipitations before performing longer term simulations with different evolutions in emissions scenarii.

Emissions de N2O en Afrique

Projet démarré en 2019

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Claire Delon**

RegCM-CLM coupled models are mainly developed by ICTP (International Center for Theoritical Physics) and NCAR (National Center for Atmospheric Research), but also by the Laboratoire d'Aérologie with Fabien Solmon among others. This model is used to simulate numerous environmental and meteorological parameters as well as bio-geophysical and chemical dynamics of the soil such as N2O emissions. N2O is an important greenhouse gas (300 times more powerful than CO2) and has also an impact on ozone depletion in the stratosphere. This gas is studied in the framework of projects focused on the nitrogen cycle at the Laboratoire d'Aérologie. For now, N2O emissions from soils as been encoded into RegCM-CLM model but has neither been tested nor been developed for the

moment. The aim of this project is to compare RegCM-CLM simulations of N2O emissions from soils with our observation data and to improve the code if necessary. N2O production in soil is highly dependant on numerous environmental parameters, particularly on carbon and nitrogen content in soil. However, the model needs numerous years of simulation before reaching a stable amount of carbon and nitrogen content from year to year. This stabilisation is important if we want to compare the simulation results with our data as we need to be sure that the variations are due to realistic environmental conditions and not to an unsteady state of the model. We therefore need to launch a 200 years spin up with the same meteorological year to verify if a carbon and nitrogen threshold in soil is reached. This simulation will then be used as an initialisation for our future simulations. This is why we would like to use this CALMIP opportunity to go further in our work.

Compréhension de la matière dans les étoiles à neutrons

Projet démarré en 2019

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Natalie Webb**

As massive stars end their life in supernova explosions, their inner core collapses to incredible densities to form neutron stars (NS), the densest objects known in the Universe. Fifty years after the discovery of NS, the behaviour and composition of the ultra-dense matter in their core remain unknown. Since such extreme densities cannot be reproduced in Earth laboratories, astrophysical observations of NS provide the only manner to discriminate between the many theoretical models of nuclear physics that attempt to describe ultra-dense matter. Understanding the behaviour and composition of such matter represents one of the main goals of nuclear physics, since it would improve our understanding of quantum chromodynamics. In addition, this has tremendous implications for the astrophysics of supernova explosions and for the coalescence of NS (emission of gravitational waves, etc.) A handful of methods exists to constrain models of ultra-dense matter from observations of NS and the most promising techniques involve determining their masses M and radii R. This permits direct comparison of such measurements with the M-R relations predicted by theoretical models. One novel method for M and R measurements exploits the data collected by the Neutron Star Interior Composition ExploreR (NICER), an X-ray observatory installed in June 2017 on the International Space Station. NICER's main goal is to observe X-ray emitting NS to measure their M and R. These objects emit X-rays from small hot polar caps which cause flux variations as the NS rotate. Modelling these flux variations permits obtaining measurements of the NS compactness, i.e., M and R. However, the model calculation, which requires modelling the surface emission and the space-time surrounding the NS, depends on many parameters, and requires computationally intensive parameter estimations. This proposal requests the computation time necessary to extract the M and R of the NS for which we have acquired data with NICER.

Inversion de formes d'onde altimétriques

Projet démarré en 2019

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Fernando NIÑO**

Since July 2018, we have set up an altimetry waveform inversion tool in the laboratory: using radar data from altimetry satellites and a simulator of these data, we are able to build databases of altimetry waveforms (the radar echoes) from which we apply machine learning techniques with deep networks. The methodology foresees two distinct phases: the generation of simulated data from our simulation code (written in python with a computational core in C), then the integration of these data into the neural network as a learning database . Today the network performances are very good for altimetry data in hydrology, but less well in the coastal area, more

complex. We need to increase the number of data in the learning base, and create a new neural network with these new data. Today we mainly use a linux PC equipped with a GPU GTX 1080, but it is insufficient for the type of application envisaged. We have already used the CNES cluster, with good results, but it still has only 4 GPUs, and the demand is such that they are already completely saturated. This project aims to deploy on Calmip all the software infrastructure of simulation and deep learning, and establish if the use of this methodology can improve in the coastal domain, and to produce some results that can confirm calculations indicating the precision that can be reached. The coupling of the alimetric simulation with high-resolution oceanic models, is done with Symphonie which has already ran in Calmip.

Interaction aerosol nuage bas et climat regional dans le sud Est Atlantique, AEROCLO-sA

Projet démarré en 2019

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Fabien Solmon**

The AEROCLO-sA (AErosol, RadiatiOn and CLOuds in southern Africa) project investigates the role of aerosols on the regional climate of southern Africa. This is a unique environment where natural and anthropogenic aerosols and a semi-permanent and widespread stratocumulus (Sc) cloud deck are found. The project aims to understand the dynamical, chemical and radiative processes involved in aerosol-cloud-radiation interactions over land and ocean and under various meteorological conditions. Part of the project consist in characterizing these interactions using modelling approaches constrained by experimental data collected during AEROCLO-sA. Laboratoire d'Aérologie is in charge of running regional climate simulation experiments to quantify above cloud radiative forcing and its variability over decadal time scales, explore the cloud properties modification induces by this radiative forcing, and characterize the effective regional climate impact of biomass burning aerosol.

Modélisation sismique des étoiles sous-géantes

Projet démarré en 2019

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Sébastien Deheuvels**

Asteroseismology, which consists in studying the oscillations of stars, is currently the only tool to probe stellar interiors. The recent development of space missions partly dedicated to asteroseismology, such as CoRoT, Kepler, TESS, and soon PLATO, has opened a golden age for this discipline and has already led the community to revisit several open questions in stellar physics. The seismology of subgiants is particularly rich. Stars reach this stage when the hydrogen content in their core is exhausted. Then, the core contracts while the envelope expends (hence the name "subgiants"). From a seismic point of view, these stars oscillate following so-called "mixed" modes, which behave as pressure modes in the envelope and as gravity modes in the core. These modes make it possible to probe the deep stellar core, which is generally out of reach in other stars. Our project consists in exploiting subgiants to make progress in one of the most challenging open questions in stellar physics, which is the size of convective cores. For stars that possess a convective core, having a precise knowledge of the extent of the core is crucial because it play the role of a reservoir for the nuclear reactions. It is now well known that several poorly-understood physical processes can extend the size of convective cores (such a s core overshooting). This constitutes one of the main sources of uncertainty for stellar ages. We have already shown that mixed modes in subgiants can be used to measure the size of convective cores and we have developed a seismic modeling method for this purpose (Deheuvels & Michel 2011). We now wish to apply this method to subgiants observed with Kepler. This involves the computation of numerous stellar evolution models in parallel, for which we require computing time at CALMIP.

Modeling of tropical cyclone activity in the Eastern Pacific basin – Sensitivity to oceanic stratification

Projet démarré en 2019

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Lionel Renault**

A wide modeling effort, relying on collaborations at LEGOS and MERCATOR and a PhD trainee, will be carried out to quantify the upper-ocean contribution to the Tropical Cyclone activity in the Eastern Pacific. The use of long basin scale simulations is expected to bring in-depth understanding of the influence of different modes of oceanic variability on the hurricane seasonal activity in the Eastern Pacific basin. To do so high-resolution coupled simulations will be performed using (CROCO1⁄12°-WRF1⁄6°). The use of different initial conditions, forcing (climatological vs. specific ocean setting), vertical parameterizations (different stratifications, deep vs. shallow mixed layer) will allow refining our understanding of ocean processes linked to storm intensification within different ocean dynamical backgrounds.

Atmospheres Stellaires

Projet démarré en 2019

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Michel Rieutord**

On souhaite tester le code de calcul PHOENIX qui permet de calculer la structure d'une atmosphère stellaire ainsi que le spectre émis. Ce code est parallélisé MPI.

Darwin

Projet démarré en 2018

EcoExMoulis - Station d'Ecologie Expérimentale (USR 2936)

Porteur de projet: **Jose Maria Montoya Teran**

Climate change is a global phenomenon whose effects pervade all biomes, from the tropics to the poles. Different biomes, however, are affected at different rates of change, and the characteristics of the local ecosystems, in particular species interactions, can ameliorate or exacerbate the ecological consequences of climate change. Thus, one of the greatest challenges of this project is to investigate how local differences in both the environmental stressors and biotic interactions modulate the effects of climate change. Marine phytoplankton play a critical role in marine food web, global biogeochemical cycles and climate processes, making them important indicators for ecosystem state under climate change. Thus, we use a global ecosystem model combined with ocean circulation model to gain mechanistic insights into how changes in species interactions modify global distribution patterns of plankton species across spatial scales and how future climate change affects the marine ecosystems worldwide.

Modélisation des jets zonaux dans les océans équatoriaux

Projet démarré en 2018

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Yves Morel**

The request for opening a project at CALMIP for our study is motivated by the need to implement high resolution ocean basin scale simulations using the CROCO (Coastal and Regional Ocean Com munity Model) numercial model. This model solves the primitive equations from small scale fluid mechanics to geophysical flows. It is developed by a consortium of French laboratories, including LEGOS and LA in Toulouse. This model is capable of modeling all scales of fluid mechanics (from turbulence to global circulation of the ocean). It is parallelized and optimized for multiprocessor computing. Our project is a process study related to equatorial ocean circulation. The aim is to identify the mechanisms involved in the creation of deep jets recently observed in the ocean circulation of the tropical / equatorial band. Our goal is to test various configurations, forcings and parameters of a simplified ocean model to understand the origin of these jets, which are currently not properly described in realistic models of the ocean.

Modélisation de la dynamique et de la chimie atmosphérique à mésoéchelle : chimie en phases gazeuse, aqueuse et aérosols

Projet démarré en 2018

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Céline Mari**

This project aims at understanding the dynamical and chemical processes which control the atmospheric composition, clouds and dynamics with the Meso-NH model and machine learning methods. The french ANR TTL-Xing project is devoted to the study of the impact of monsoon convection on the composition of the UTLS and on the formation of the Asian Tropopause Aerosol Layer (ATAL). High resolution simulations with the Meso-NH cloud resolving model in the Asian monsoon region will be performed to explicitly represent convective clouds and associated processes (scavenging of particles, aerosol-cloud interactions and in-cloud chemistry). The objective is to document the preferential transport processes (fast convective uplift versus slow diabatic heating) and the geographical origin of the pollutants. The high resolution Meso-NH simulations will be performed for case studies observed during the StratoClim 2017 monsoon campaign. The MOPGA EUROACE project aims at improving the roles of aerosols in climate and environment with a focus on aerosol-cloud interactions. More specifically, the role of anthropogenic aerosols on cloud microphysical structure and lifetime will be studied with cloud scale and LES simulations with the Meso-NH model, enriched with a new aerosol model MARC, and machine learning methods. Probabilistic collocation Methods (PCM) and deep machine learning will be used to derive new parameterizations of processes in aerosol-cloud interaction. In particular, the project will experiment deriving the arguably most challenging parameterization for aerosol-deep convection interactions (from aerosol processing and redistributing to aerosol-cloud microphysical connections) using deep learning algorithms based on a large quantity of LES model outputs combined with observations of deep convection systems.

Dernières publications:

- Brosse, F ; Leriche, M ; Mari, C ; Couvreux, F., LES study of the impact of moist thermals on the oxidative capacity of the atmosphere in southern West Africa, ACP, doi :10.5194/acp-18-6601-2018, 2018 - **doi:** pu.doi

Non-hydrostatic modelling investigations over the strait of Gibraltar

Projet démarré en 2018

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Laurent Roblou**

The Mediterranean Sea is a semi-enclosed basin featuring an active thermohaline circulation that is maintained by the atmospheric forcing and regulated by the Strait of Gibraltar. Briefly, over the Mediterranean Sea, the ocean-atmosphere fluxes are balanced by the exchange flow that takes place within the strait of Gibraltar. Within the strait, the ocean circulation features a two-way exchange, directly influenced by the interaction between the intense tidal forcing and the complex geometry of the strait, through the mixing mechanism due to internal tides and a hydraulic control. Some aspects of the strait hydrodynamics could not be well reproduced by standard numerical model. This especially concerns the evolution of the internal tidal bore generated in the main sill area. After its generation, the bore progresses toward the Mediterranean, evolving into a series of short internal solitary waves of large amplitude. These waves are strongly nonlinear and nonhydrostatic, thus their modeling requires fully nonhydrostatic codes such as the new-generation ocean modelling system CROCO (www.croco-ocean.org) from the Coastal and Regional Ocean Community (GdR CROCO). This feature is essential and necessary to perform regional ocean LES. Thus, the main goal of this proposal is the investigation of several open questions on the hydraulic behavior of the strait of Gibraltar applying the nonhydrostatic assumption, AGRIF grid refinement and new monotonic implicit large eddy simulations (MILES) parameterizations. Specifically, the evaluation of the impact of these novel features on the internal solitary waves forced by the tides in the strait of Gibraltar is one of the scopes of this proposal. The present study is a component of the exploratory effort that will lead to the in-situ campaign GIBRALTAR2020. In this framework, in the continuity of the P18017 grant, the project team is applying for 210 000 hours of computing time and associated data storage on the CALMIP platform.

Gravity field and tidal deformations of small bodies of the solar system

Projet démarré en 2018

ISAE/DEOS - Département Electronique, optronique et signal

Porteur de projet: **Raphael Garcia**

As elementary bricks of planets, asteroids are a special target of interest for scientists in order to grasp a better understanding of the early Solar system formation and therefore determining the internal structure of planets and small bodies. Several space missions with asteroids as their main goal have already been launched and more are planned to follow suit. Therefore there is a real need to improve our models of asteroids for the smooth progress and planning of these missions. For this project, we choose to focus on the gravity field and seismic measurements among the available observables for asteroids: the gravity field having already been measured and being essential for missions getting closer to asteroids, and seismic measurements as it is one of the most efficient ways to determine the internal structure of celestial bodies. The aim of this project is to determine the global gravity field of any asteroid, their tidal deformations and potential sources of seismic waves. Especially, we study the tidal forces exerted upon an asteroid so that tidal displacements, and thus tidal stress, can be calculated. This gives us information about the stress state of the asteroid and if material failure is likely to happen, which would mean tidal quakes happening and thus allowing passive seismology at the surface of these bodies. Because of the highly diverse shapes and internal structure of asteroids, standard methods used on almost spherical bodies cannot be applied here, and specific numerical methods are required. This project will use and expand the library FreeFEM++ for solving gravity field and tidal deformations of small objects of the solar system.

SenSAgri

Projet démarré en 2018

CESBIO - Centre d'Etudes Spatiales de la BIOsphère (UMR 5126)

Porteur de projet: **Eric Ceschia**

Our team is part of the Sentinels Synergy for Agriculture (SenSAgri) project that is financed by the European Commission. The goal of this project is to develop an innovative portfolio of prototypes agricultural monitoring services. In this project, our team focuses on the development of a processing chain that construct dynamic crop maps of the land usage updated regularly over the agricultural season. Those maps are created from the Sentinel satellite image series and in-situ field data by using supervised classification algorithms. One of our main goals is to be able to construct those maps as soon as possible during the agricultural season [1]. The new satellite images acquired by Sentinel mission initiate a new area in Earth Observation. As main novelty, Sentinel mission provides systematic global acquisitions of high-resolution multi-spectral and radar imagery with a high revisit frequency, [2]. The use of both radar and optical data in synergy is the main motivation of the SensAgri project. The complementarity of both sources of information allows accurate land cover discrimination. Therefore, the generation of accurate maps is possible thanks to this huge amount of information. However, the processing of these large data volumes requires an important number of computational resources. The first classification experiments of Sentinel images times series have been performed by using a processing chain prototype, which has been developed at CESBIO. The main programs are developed in C++ and they are interfaced with Python. In the last year, thanks to CALMIP resources, the chain has been successfully tested on different test sites in Europe, representing a surface of more than 100000 km². Our goal to evaluate the proposed methodology on a large scale have been successful. In 2019, we will have to perform similar tasks on the same test sites but for the agricultural year of 2018. New test sites will be considered in Ukraine, South Africa and Argentina adding about 60000km² to the surface to analyze. To perform those tasks, we still want to use CALMIP resources.

Modélisation numérique directe du mélange de traceurs océaniques

Projet démarré en 2017

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Yves Morel**

The general context of the project is the TEASAO IDEX project which aims at the preparation of the next generation of prediction systems for both the atmosphere and the ocean. A major scientific challenge to do so is to improve understanding and modelling of the effect of small-scale turbulence and vertical mixing on the evolution of chemical or biological species in both the ocean and the atmosphere and its integrated effect at larger scales. This has strong relevance for societal problems such as fresh water resources, air or water quality, pollution development and spreading, primary ocean production (plankton) and fisheries. Many of the outstanding scientific questions in this area are common to both ocean and atmosphere and the rationale for the TEASAO project is that there is much to be gained by the atmosphere and ocean scientific communities in Toulouse from exploiting this commonality. The project is based on the long-term visit of Professor Peter Haynes, from University of Cambridge (UK), who is an international expert on the dynamics of atmosphere and ocean and on the transport and mixing of trace species, including reacting chemical and biological species. The project is built with an original combination of theoretical to applied studies. One scientific goal of the TEASAO project is thus to build a common framework to address the theoretical aspects of the evolution of active tracers in turbulent stratified flows, in particular the evolution of their distribution along density classes. Data and more realistic applications will be provided by specific studies for the ocean (plankton growth in along an upwelling front) and for the atmosphere (the interaction between turbulence, mixing and microphysics on different scales in the tropical tropopause layer). The global expected fallouts for Toulouse are cohesion and visibility, on a subject at the frontier of the present scientific concerns, and the preparation of the next generation operational systems for both the atmosphere and the ocean. The TEASAO project will also benefit the local higher education programs and several actions are planned with this perspective.

TROLL

Projet démarré en 2017

EDB - Évolution et Diversité Biologique (UMR 5174)

Porteur de projet: **Jerome Chave**

We have developed an individual-based forest growth simulator to model the dynamics of carbon in a tropical forest ecosystem but also to jointly monitor its biodiversity. This model TROLL, offers unique potentialities to constrain global dynamic vegetation models, that are now commonly coupled with climate models in Earth System Models. We have assembled a long-term knowledge of tropical forests of French Guiana and aim to implement this strategy as part of the activities of Labex CEBA. Specifically, we propose to (1) improve TROLL by including the carbon, water, and nutrient balances, and including a species-level parameterization of the main plant-level processes for the tropical forest of French Guiana; (2) mobilize high-resolution remote-sensing data (aerial LiDAR scanning) to inform plant allometry and canopy structural properties, as well as topographical features; (3) mobilize forest dynamic data to validate the model, implement a forest management module and a forest fire module; (4) as a exercise of the model's scaling properties, scale-up the simulations to the entire area of French Guiana (c.a. 84,000 km2) making use of recent progress in our understanding of tree species distribution and ecological processes at this scale; (5) provide scenarios to assess the impacts of land use change, forest management and climatic change on selected forest types of French Guiana. The findings of this project should have an impact beyond French Guiana, in other Neotropical forests. It should also provide to the scientific community of Labex CEBA a modeling tool to assimilate information from several research lines (forest ecology, remote sensing, climate science, socio-economics), and suggest optimal development paths for the coastal forests for regional policy and local managers of natural areas, who are faced with practical challenge of maintaining wood production while protecting biodiversity and carbon stocks.

Dernières publications:

- Maréchaux, I., & Chave, J. (2017). An individual-based forest model to jointly simulate carbon and tree diversity in Amazonia: description and applications. Ecological Monographs. -
- Fischer, F. J., Maréchaux, I., & Chave, J. (2019). Improving plant allometry by fusing forest models and remote sensing. New Phytologist. -

Characterizing stellar parameters from high resolution spectra of mature and young low-mass stars

Projet démarré en 2017

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Jean-François Donati**

Observational studies in stellar physics critically depend on having well constrained and homogeneous sets of fundamental parameters for all stars in the studied samples; this is particularly true for radial velocity (RV) studies aimed at characterizing orbiting planets, or spectropolarimetric studies whose goal is to investigate stellar magnetic topologies. Whereas stellar parameters of FGK main sequence (MS) stars can be reliably estimated with a number of existing tools (eg iSpec, SME), the task gets significantly more complex for M dwarfs and young pre-MS stars, for which existing stellar spectral libraries are much less accurate and struggle to accurately describe the wealth of observed molecular lines, especially in the near infrared (nIR) where even line parameters of atomic lines are poorly constrained. We propose to generate a high-resolution optical & infrared spectral library, to be made available to the community ultimately, using PHOENIX model atmospheres (Allard et al, 2011, ASPC 448, 91) that are presumably the best option in terms of physical realism for cool stars atmospheres and the modeling of molecular lines. The grid of stellar parameters we will explore for M dwarfs spans 2500 to 4500 K for the temperature (w/ steps of 25 K), 3.5 to 5.5 for the logarithmic gravity (w/ steps of 0.05), and -1 to 1 for the metallicity (w/ steps of 0.05). We will use this spectral library to accurately characterize stellar parameters of a

sample of M dwarfs (w/ masses in the range 0.1-0.5 Msun) and those of a sample of low-mass PMS stars (0.3-1.0 Msun) currently observed with SPIRou, the new high-resolution nIR velocimeter and polarimeter installed on the Canada-France-Hawaii-Telescope (CFHT) in 2018 and whose science observations started in 2019.

Dernières publications:

- SF2A-2017: Proceedings of the Annual meeting of the French Society of Astronomy and Astrophysics - **url:** pu.open_url
- Kulenthirarajah L, Donati JF, et al, MNRAS, in press -

Signatures observationnelles de la migration planétaire dans les poussières des disques protoplanétaires

Projet démarré en 2016

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Clément Baruteau**

Planets form in a protoplanetary disc of gas and dust surrounding young stars. The gravitational interaction between planets and the gas component of their protoplanetary disc can decrease or increase the distance between planets and their star, at a pace that depends on the planet mass and the physical properties of the disc (density, temperature etc.). This is known as planetary migration. It plays a prominent role in our understanding of the orbital properties of extrasolar planets, and of the observations of protoplanetary discs, for which the extremely diverse gas and dust distributions (spirals, rings, lopsided asymmetries etc.) are often interpreted as signatures of planets buried in the discs. However, contrary to the gas component of protoplanetary discs, planet-disc interactions in the dust remain largely unknown. In particular, the implications of planetary migration on the spatial distribution of the dust in protoplanetary discs have never been investigated. This is the scope of this application for CalMip computing time. In this project, I will carry out hydrodynamical simulations modelling both the gas and dust components of a protoplanetary disc where a planet forms. Numerical simulations will make use of the public hydrodynamical code Fargo to which I have recently implemented a dust particle integrator (tested, validated and published). The planet's mass and the disc's physical properties will be varied to explore various regimes of planetary migration. Their impact on the distribution of dust grains of various sizes will be examined. Inclusion of several planets is also anticipated in this project. The results of simulations will be used to produce synthetic images of the dust continuum emission as it would be observed via interferometric imaging (like with the ALMA telescope).

Dernières publications:

- Baruteau, Barraza, Pérez, Casassus, Dong, Lyra, Marino, Christiaens, Zhu, Carmona, Debras & Alarcon 2019, "Dust traps in the protoplanetary disc MWC 758: two vortices produced by two giant planets?", MNRAS, 486, 304-319 - **doi:** pu.doi
- Pérez, Casassus, Baruteau, Dong, Hales & Cieza 2019, "Dust unveils the formation of a mini-Neptune planet in a protoplanetary ring", AJ in press - **doi:** pu.doi

Magnetisme des amas (MAMAS)

Projet démarré en 2016

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Francois Rincon**

This project aims at investigating the effects of convective fluid instabilities such as the magnetothermal (MTI) and heat flux buoyancy driven (HBI) instabilities in galaxy clusters. These instabilities are thought to contribute to

the magnetisation of the intracluster medium (ICM) and extragalactic plasmas, and may also provide a significant non-thermal pressure support to the ICM, with potentially important implications for cosmological studies relying on clusters. As a first step, in 2016 we developed new functionalities in the MHD code SNOOPY, in order to be able to perform high-resolution simulations including the effects of anisotropic heat conduction and Braginskii viscosity on the stability of stratified magnetised plasmas. We also performed a preliminary scan of parameter space for 3D simulations. We now plan to extend these simulations to higher resolution in order to assess the effects of dissipative processes on the MTI and HBI, to characterise carefully how they may affect heat transport and induce magnetic field in clusters, and to quantify the pressure support associated with the subsequent turbulence, with the goal of improving phenomenological dynamical and thermodynamical models of galaxy clusters.

Modélisation des environnements ionisés

Projet démarré en 2015

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Pierre-louis Blelly**

The Magnetosphere / Ionosphere / Thermosphere (MIT) system plays a critical role in the Sun-Earth connections and it is a key element in Space Weather. The couplings between the three different subsystems are a complex mix of fluid / kinetic transport, chemistry and electrodynamics with charged particles trapped in the background magnetic field and the three regions are so deeply intricated that deconvoluting the various interactions is a tough challenge in view of developping any service dedicated to Space weather. The project aims to focus on some aspects of these couplings. Especially, we wish to study the interactions within the plasmasphere, which is the inner part of the magnetosphere. For that, we have developped a time dependent numerical model which is able to solve the interhemispheric dynamics of the ionospheric plasma along convecting magnetic field lines inside the plasmasphere. This code has been parallelized so that we can follow a large number of flux tubes at different locations (~2000) and thus we can reconstruct the 3D motion of the ionospheric plasma. Such an approach is rather innovative in the sense that this model has a high resolution along the magnetic field line and accounts for a large number of processes controlling the lower part of the ionosphere. We are interested in the steady state equilibrium of the plasmasphere that could arises from such a convecting model because it provides background conditions for the inner magnetosphere stability. For that, we want to model the plasmasphere for different solar illumination cases : solstice, equinox, high solar activity, low solar activity, ... and follow the dynamics of the plasma between the two hemispheres with a focus on the magnetic equatorial plane.

Dernières publications:

- Beatriz Sánchez–Cano, Pierre-Louis Blelly, Mark Lester, Olivier Witasse, Marco Cartacci, Roberto Orosei, Hermann Opgenoorth, Robert Lillis, François Leblanc, Stephen E. Milan, Philip Conroy, Nicolas Floury, John M. C. Plane, Andrea Cicchetti, Raffaella Noschese, Andrew J. Kopf, Origin of the Extended Mars Radar Blackout of September 2017, J. Geophys. Res., 124, 4556-4568, doi:10.1029/2018JA026403, 2019. - **doi:** pu.doi
- Aurélie Marchaudon and P.-L. Blelly, Impact of the dipole tilt angle on the ionospheric plasma as modeled with IPIM, submitted to JGR, 2019. - **doi:** pu.doi

Assombrissement gravitationnel des étoiles à enveloppe convective

Projet démarré en 2015

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Michel Rieutord**

This project focuses on the problem of gravitational darkening of rapidly rotating stars with an outer convective envelope. For this, we shall examine the dependence of the convective flux on latitude for a set of simplified models made of a rotating spherical layer heated from below. We use direct numerical simulations of this set-up with the code MAGIC that solves the hydrodynamic equations with a pseudo-spectral method based on Chebyshev polynomials and spherical harmonics. The point is to explore the range of parameters reachable with a DNS and then devise models that can be applied to the extreme (in terms of numbers) case of stars.

Dernières publications:

- Raynaud R., Rieutord M., Petitdemange L., Gastine T. and Putigny B. (2017), "Gravity darkening in late-type stars. I Coriolis effect", in Astron. & Astrophys. vol. 609, A124 - **doi:** pu.doi
- Raynaud R., Rieutord M. and Gastine T. (2020), "Gravity darkening in late-type stars. II Centrifugal effect", en préparation pour Astron. & Astrophys. -

Structure et dynamique du vent solaire lent

Projet démarré en 2015

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Alexis Rouillard**

This project addresses the outstanding problem of the origin of strongly twisted magnetic flux-tubes detected by spacecraft in the slow solar wind streams. These are coherent structures extend, in principle, from the lower layers of the solar atmosphere up the the interplanetary space. Their origin remains illusive, at present date, even though a few competing hypothesis have been proposed. These rely on magneto-hydrodynamical processes whose effects have not yet been properly quantified and confronted with observations. Beyond the problem of their origin, the actual dynamics of these magnetic structures are still misunderstood (e.g, are these transient Alfven-like wavefronts or large-scale quasi-stationnary structures?). This is a key issue for the Space Weather activities, as the dynamics of these magnetic structures affects the way solar surface perturbations are propagated up to the Earth environment. This proposal relies on a well-tested 3D MHD numerical setup tailored for the purpose and based on the PLUTO code (with excellent MPI scaling and perfectly adapted to massively parallel computing environments) and on PIC simulations using the code SMILEI.

Dernières publications:

- Kouloumvakos, A., Vourlidas, A., Rouillard, A.P.,..., The solar origin of particle events measured by Parker Solar Probe during second encounter, Submitted to ApJ, 2019 -
- Wu, Y., Rouillard, A.P., Kouloumvakos, A.,..., Origin of the type-II radio burst and hard X-Ray Emissions during the 1 September 2014 event, Submitted to ApJ, 2019 -

Assimilation SWOT SURFEX

Projet démarré en 2014

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Sylvain Biancamaria**

The future SWOT (Surface Water and Ocean Topography) satellite mission, jointly developed by NASA and CNES for a proposed launch around 2020, will provide 2D maps of ocean and continental water bodies surface elevations. This mission will therefore provide unprecedented information on the seasonal and spatial variability

of the continental water cycle at global scale. Currently, hydrological models (like ISBA-TRIP which is part of the SURFEX platform developed at CNRM) are commonly used to study the global continental water cycle. However, it is extremely difficult to gather global datasets to estimate all of the parameters needed for such hydrological models (such as river depth/width, friction coefficientï¿½) and are currently approximated using empirically-based parametrizations. Yet, this is the kind of information which can be derived from SWOT. Thus the goal of our overall project, mainly based at LEGOS, is to investigate the potential of SWOT measurements to improve parameter specification and their spatial distribution for a coupled hydrological-routing model, using data assimilation techniques. An Extended Kalman Filter has already been developed at CNRM to assimilate virtual SWOT observations into ISBA-TRIP to correct friction coefficient. The purpose of the CALMIP project is to do some sensitivity analysis of ISBA-TRIP, run this assimilation platform and assess the needed improvement (on the code, but also if the assimilation scheme needs to be upgraded to an Ensemble Kalman Filter and the issue of correcting other model parameter as the bankful depth). This project will be done at LEGOS in collaboration with CNRM and CERFACS.

Dernières publications:

- Emery C., S. Biancamaria, A. Boone, P.-A. Garambois, S. Ricci, M. Rochoux and B. Decharme. "Temporal Variance-based Sensitivity Analysis of the River Routing Component of the large scale hydrological model ISBA-TRIP: Application on the Amazon Basin". Journal of Hydrometeorology, 17(12), 3007-3027 - **doi:** pu.doi
- Emery C., A. Paris, S. Biancamaria, A. Boone, S. Calmant, P.-A. Garambois, J. da Silva. "Large scale hydrological model river storage and discharge correction using satellite altimetry-based discharge product". Hydrology and Earth System Sciences, 22, 2135-2162 - **doi:** pu.doi **url:** pu.open_url

Modelling Infrasounds from Solid/Atmosphere Coupling and Applications

Projet démarré en 2014

ISAE/DEOS - Département Electronique, optronique et signal

Porteur de projet: **Raphael Garcia**

Low-frequency events such as tsunamis generate acoustic and gravity waves which quickly propagate in the atmosphere. Since the atmospheric density decreases exponentially as the altitude increases and from the conservation of the kinetic energy, those waves see their amplitude raise (to the order of 10^5 at 200km of altitude), allowing their detection in the upper atmosphere. Various tools have been developed through years to model this propagation, such as normal modes modeling or to a greater extent time-reversal techniques, but none offer a low-frequency multi-dimensional atmospheric wave modelling. A modeling tool is worthy interest since there are many different phenomena, from quakes to atmospheric explosions, able to propagate acoustic and gravity waves. In order to provide a fine modeling of the precise observations of these waves by GOCE satellite data, we developed a new numerical modeling tool. Starting from the SPECFEM program that already propagate waves in solid, porous or fluid media using a spectral element method, this work offers a tool with the ability to model acoustic and gravity waves propagation in a stratified attenuating atmosphere with a bottom forcing or an atmospheric source. Atmospheric attenuation is required in a proper modeling framework since it has a crucial impact on acoustic wave propagation. Indeed, it plays the role of a frequency filter that damps high-frequency signals. The bottom forcing feature has been implemented due to its ability to easily model the coupling with the Earth's or ocean's surface (that vibrates when a surface wave go through it) but also huge atmospheric events. Applications span from tsunami and/or atmospheric explosions detection on Earth to remote seismology when studying other solar system planets. Indeed, understanding these kind of events would eventually give the opportunity to avoid using ground seismometers when atmospheric conditions are too rough to properly settled down ground stations.

Dernières publications:

- A. Spiga et al., "Atmospheric Science with InSight," Space Sci. Rev., vol. 214, no. 7, p. 109, Oct. 2018. - **doi:** pu.doi
- L. Martire et al., "Numerical Simulation of the Atmospheric Signature of Artificial and Natural Seismic Events," Geophys. Res. Lett., Nov. 2018. - **doi:** pu.doi

Modélisation des écosystèmes planctoniques en Méditerranée

Projet démarré en 2013

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Caroline Ulses**

The objective of the project is to study the coupling of hydrodynamic and biogeochemical processes in the Mediterranean basin. The project is linked with another project about the study of the variability of physical processes in the Med Sea. Here we intend to do simulations of the impact of physical processes on the planktonic development. More precisely, the project is dedicated to establish budgets of biogenic elements and to study how the planctonic ecosystem is shaped by hydrodynamics. It aims particularly at: (i) Characterizing the history of the thermodynamic and biogeochemical properties of the water masses in a wide range of scales (from the event to the annual cycle and interannual variations and from the submesoscale to the scale of the basin), (ii) Understanding how the ecosystem is shaped by hydrodynamics in the temporal dimension and in the spatial dimension, (iii) Calculating budgets of biogenic elements in relation with water masses formation (iv) Evaluating the flux of CO2 and O2 at the ocean-atmosphere interface (v) Studying the impact of environmental changes on the variability of biogeochemical cycles

Dernières publications:

- Moullec F., Barrier N., Drira S., Guilhaumon F., Marsaleix P., Somot S., Ulses C., Velez L., Shin Y.-J., 2019. An End-to-End Model Reveals Losers and Winners in a Warming Mediterranean Sea, Frontiers in Marine Science, 6, 345, 10.3389/fmars.2019.00345 -
- Moullec, Fabien & Velez, Laure & Verley, Philippe & Barrier, Nicolas & Ulses, Caroline & Carbonara, Pierluigi & Esteban, Antonio & Follesa, Maria & Gristina, Michele & Jadaud, Angélique & Ligas, Alessandro & Diaz, Eduardo & Maiorano, Porzia & Peristeraki, Panagiota & Spedicato, Maria Teresa & Thasitis, Ioannis & Valls, Maria & Guilhaumon, Francois & Shin, Yunne-Jai. (2019). Capturing the big picture of Mediterranean marine biodiversity with an end-to-end model of climate and fishing impacts. Progress in Oceanography. 102179. 10.1016/j.pocean.2019.102179. -

Modélisation océanique à haute résolution en Mer Méditerranée

Projet démarré en 2013

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Patrick Marsaleix**

A phase-resolved wave model is derived from an ocean circulation model for the purpose of studying wave-current effects in nearshore zones. One challenge is to adapt the circulation model to the specificities of wave physics. This mainly concerns the consideration of non-hydrostatic effects and the parametrization of wave breaking. The non-hydrostatic pressure is calculated using the artificial compressibility method (ACM). The ACM-induced errors on wave dispersion properties are examined in detail in the context of the linear theory using idealized test cases. The possible compromise between the precision achieved on non-hydrostatic physics and the adjustable CPU cost

of the ACM method is looked at in detail. The modification of the wave characteristics by the bathymetric slope and the breaking of waves are then examined from a linear slope beach laboratory experiment. Finally the model is evaluated on the issue of rip currents and their feedback on the wave field using a laboratory experiment of a beach with a bar intersected by channels. This projet is developped in the frame of the LEFE "NUMEROFIX" program. The main objective of the NUMEROFIX project is to improve the representation of not explicitely resolved turbulence in circulation ocean models. The frame of the project is the mediterranean sea. Model outputs are compared to in situ measurements of turbulence (Gulf of Lion, Med. Sea) performed by the Marseille university. I am in charge of the numerical simulation of the 3D high resolution model of the NorthWestern Mediterranean sea.

Dernières publications:

- Seyfried, L., Estournel, C., Marsaleix, P., Richard, E., 2019. Dynamics of the North Balearic Front during an autumn tramontane and mistral storm: air–sea coupling processes and stratification budget diagnostic. Ocean Sci., 15, 179-198, https://doi.org/10.5194/os-15-179-2019 - **doi:** pu.doi **url:** pu.open_url
- Léo Seyfried, Patrick Marsaleix, Evelyne Richard, and Claude Estournel, 2017. Modelling deep-water formation in the north-west Mediterranean Sea with a new air–sea coupled model: sensitivity to turbulent flux parameterizations Ocean Sci., 13, 1093-1112, https://doi.org/10.5194/os-13-1093-2017 - **doi:** pu.doi **url:** pu.open_url

Regional Climate and Atmospheric Chemistry Interactions in the Mediterranean Basin

Projet démarré en 2013

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Fabien Solmon**

The evolution of anthropogenic and natural particles and gases emissions is expected to generate in fine outstanding climate and health changes (climate warming, precipitation regime changes, degradation of public health and ecosystems …). It is now necessary to address more in detail the issue of the characterization of spatial and temporal scales of particles and gases emissions, their transport in the atmosphere and their impacts. The project team has both knowledge and long-time expertise to study these various aspects through a regional modelling of the physical and chemical variability of the atmosphere using the regional climate model RegCM (Giorgi et al., 2012). Building this regional climate modelling needs long term (10+ years) and high resolution (15km) numerical simulations of the emission and the transport of gases and particles in the atmosphere. At the regional scale, the Mediterranean basin is located at the crossroads of air masses carrying gas phase species such as ozone and precursors, as well as natural (desert dust, sea-salt, SOA) and anthropogenic (black carbon, sulphate, etc.) particles. These species contributes to regional pollution and can have strong effects on the regional radiative budget with ensuing impact on regional climate fluctuations from daily to multi-decadal scales, as well as on ecosystems and air quality over the Mediterranean basin. Based on IPCC climate change and anthropogenic emission projections, the scientific objective of the MedCORDEX and ChARMEx WP7 international programs are to better quantify the possible evolution of regional aerosol and ozone budget, associated particulate matter concentrations, and aerosol radiative forcing over the Mediterranean basin. Three temporal windows are targeted for present, middle and end of the century. As part of these projects, we plan is to use the ICTP RegCM4 regional climate model including an interactive aerosol and chemistry module to perform climate-chemistry simulations over an extended Mediterranean domain. These simulations involve intense parallel supercomputing and CALMIP resources offer an ideal environment for this project. For all these reasons, the project team is applying for computing time and data storage on the CALMIP platform.

Dernières publications:

- Somot, S., Ruti, P., Ahrens, B., Coppola, E., Jordà, G., Sannino, G. and Solmon, F., 2018. Editorial for the Med-CORDEX special issue. Climate Dynamics. -

Modélisation physique et biogeochimique des estuaires en Afrique Centrale et en Asie : Application aux estuaires du Cameroun, du Gabon et du Golfe du

Projet démarré en 2013

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Thomas Duhaut**

One of the main objectives of the modelisation of hydrodynamic and biogeochemical modelisation in central Africa and Asian estuaries is to develop and test new numerical methods for coastal circulation with SYMPHONIE model which take into account mangrove forest, siltation, Sea level rise change and climate changes. This project will also help to describe the ocean circulation in east of Gulf of Guinea and Gabon who are very poor in physicals oceanography studies. This project intends to enforce the exchanges between the different teams (POC ,ECOLA) and different laboratory (LA, LEGOS). More recently we are extending our work to other estuaries in Africa (in Gabon, Benin) but also in Asia (Gulf of Tonkin, South China Sea) and we also propose to go further into biogeochemical point of view of those highly anthropologically constrainted systems. A first step is to simulate the circulation with different forcing : ocean circulation (MERCATOR,COPERNICUS), atmospheric forcing (GLORYS and ECMWF) , Tidal Forcing (FES2014) and River discharges and sediment transport in area. Circulation models on various test cases, including fully realistic cases requiring strong computing resources motivating the present request made to CALMIP.

Application d'OpenFOAM aux Transferts dans les sols

Projet démarré en 2012

GET - Géosciences Environnement Toulouse (UMR 5563)

Porteur de projet: **Laurent Orgogozo**

On continental surfaces, a part of rain waters infiltrates in soils. These direct infiltrations are among the main recharges of the groundwaters, which are the most commonly used drinkable water reservoirs. Consequently the study of water transfers through soils is an important stake for water engineering. Moreover, many other applications involve the transfer of water into soils (geotechnics, agronomics, environmental engineering, …). In geosciences, these phenomena are also of great interest for the study of continental surfaces. Infiltration of water into soils is classicaly modelled by the so-called Richards equation. A solver for Richards equation have been implemented in the framework of OpenFOAM, a CFD tool box which allows massively parallel computing. 2 publications in Computer Physics Communications present this solver (RichardsFoam2) and its parallel performances (Orgogozo et al., 2014, Orgogozo 2015). In the case of boreal continental surfaces, one need to be able to take into account the freezing/thawing of water into soils, which induce the presence of permafrost. In order to do so, a multiphysic solver, permaFoam, which solves the thermal transfers with phase changes and the water flow into soils has been developed in the framework of OpenFOAM. This solver has been presented for example at the InterPore conference 2017 and at the EUCOP 2018. The application to field data sets acquired in an experimental watershed in Central Siberia is the subject of a paper accepted in Permafrost and Periglacial Processes (Orgogozo et al., accepted). A new site of application will also be modelled in 2019: the INTERACT station of Khanimey. Connectively, a theoritical and experimental study of mosses and lichens (which cover a large part of the boreal surfaces) transfers properties has been started with IMFT. This study will require also 3D numerical calculations with important computational resources. For these purposes we need dedicated allocation of about 500 000 hours of CPU time on CALMIP for the year 2019.

Dernières publications:

- Orgogozo L., Grenier C., Quintard M., Prokushkin A.S., Pokrovsky O.S., Viers J., Audry S. Application of OpenFOAM® to permafrost modeling – the permaFoam solver. Oral presentation at the 7th ESI OpenFOAM Conference, 16th October 2019, Berlin. - **url:** pu.open_url
- Orgogozo L., Pokrovsky O.S., Grenier C., Mouche E., Marcoux M., Quintard M. High Performance Computing for permafrost modeling: towards mechanistic assessments of climate change impacts at the scale of the experimental watershed. Oral presentation at the Franco-Russian workshop "Environmental Changes in Siberia", 21st October 2019, Paris. - **url:** pu.open_url

Prévisibilté des épisodes de précipitations intenses dans la région méditerranéenne (Code Méso-NH)

Projet démarré en 2012

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Evelyne Richard**

This proposal aims at improving the predictability of heavy precipitation events that frequently hit the Mediterranean coastal regions. It is closely linked to the recent international field experiment HyMeX (http://www.hymex.org/). Our goal is to develop ensemble forecasting methologies suited for the convective scale. The work will be based upon the Meso-NH atmospheric model (http://www.hymex.org). Both initial state uncertainties and model errors will be accounted for.

Dernières publications:

- Lac, C., Chaboureau, J.-P., Masson, V., Pinty, J.-P., Tulet, P., Escobar, J., Leriche, M., Barthe, C., Aouizerats, B., Augros, C., Aumond, P., Auguste, F., Bechtold, P., Berthet, S., Bielli, S., Bosseur, F., Caumont, O., Cohard, J.-M., Colin, J., Couvreux, F., Cuxart, J., Delautier, G., Dauhut, T., Ducrocq, V., Filippi, J.-B., Gazen, D., Geoffroy, O., Gheusi, F., Honnert, R., Lafore, J.-P., Lebeaupin Brossier, C., Libois, Q., Lunet, T., Mari, C., Maric, T., Mascart, P., Mogé, M., Molinié, G., Nuissier, O., Pantillon, F., Peyrillé, P., Pergaud, J., Perraud, E., Pianezze, J., Redelsperger, J.-L., Ricard, D., Richard, E., Riette, S., Rodier, Q., Schoetter, R., Seyfried, L., Stein, J., Suhre, K., Taufour, M., Thouron, O., Turner, S., Verrelle, A., Vié, B., Visentin, F., Vionnet, V., and Wautelet, P.: Overview of the Meso-NH model version 5.4 and its applications, Geosci. Model Dev., 11, 1929-1969. - **doi:** pu.doi
- Seyfried, L., P. Marsaleix, E. Richard, C. Estournel. Dynamics of North Balearic Front during an autumn Tramontane and Mistral storm : air-sea coupling processes and stratification budget diagnostic. Ocean Sci. Discuss., https://doi.org/10.5194/os-2018-14, 2018 Revised manuscript under review for OS - **doi:** pu.doi

Simulation explicite des propriétés microphysiques des orages avec le modèle MésoNH

Projet démarré en 2011

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Jean-Pierre Pinty**

We are using our "MésoNH" tool, a highly parallelized and vectorized code of an atmospheric multipurpose non-hydrostatic research model. Our project is concerned by the cloud scheme LIMA that includes explicitly the effects of a population of aerosols of different origin. These are used here to compute the number concentrations of the cloud droplets (CCN activation process) and those of the pristine ice crystals (IFN heterogeneous nucleation) to initiate the ice phase. An issue is to illustrate the initialization of the 3D aerosol fields with the MACC II analyses

available at ECMWF, Reading, UK. In addition, our purpose is to test an enriched version of LIMA that includes two secondary production mechanisms of ice crystals by ice break-up and raindrop shattering, and that predicts also pristine ice crystal habits which are deemed to be important for accurate cloud physics and radiative transfer modeling. The simulations include: 1- 4 cases of academic midlatitude/tropical cloud systems to measure the relative importance of the secondary production processes of ice crystals according to the cloud base temperature and height of the freezing level, 2- cases of HyMeX_2012 (Gulf of Lion area) and EXAEDRE_2018 (Corsica area) to check the LIMA scheme with accurate airborne data (ice concentrations and ice crystal habits), 3- cases of HAIC experiment (Darwin_2014 and Cayenne_2015) where very high concentrations of ice crystals were recorded. Typically the 24h simulation domain is ~500x500 gridpoints with 50-760 levels. A 2-model simulation (with grid-nesting) lasts 20 hours for 250 core run.

Dernières publications:

- * Barthe, C., M. Chong, J.-P. Pinty, C. Bovalo, and J. Escobar, CELLS v1.0: updated and parallelized version of an electrical scheme to simulate multiple electrified clouds and flashes over large domains, Geosci. Model Dev., 4, 2849-2892, 2011. -
- Hoarau T., Pinty J.-P., and C. Barthe, A representation of the collisional ice break-up process in the two-moment microphysics scheme LIMA of Meso-NH, submitted to Geosci. Model Dev. - **url:** pu.open_url

CASSANDRE « Calcul Haute performance pour la modélisation de la propagation d'ondes et les méthodes potentielles »

Projet démarré en 2011

GET - Géosciences Environnement Toulouse (UMR 5563)

Porteur de projet: **Roland Martin**

In the mean term the goal will be to solve joint inversion problems on High performance multi-CPUs and multi-GPUs clusters. We identified four problems requiring high performance computing : three-dimensional efficient and fast wave propagation modelling at the regional scale (Pyrennes chain) using joint seismic and gravity inversion which should be correlated in the future with (electro)magnetic imaging. In 2018 we have been able to perform a gravity inversion of one profile through the Pyrenees chain but we would like to perform the same kind of inversion for three other transects through the Pyrenees and on Maupassacq TOTAL dense arrays. In order to extend these techniques to other zones of the Earth, we aim at applying joint gravity/seismic inversions using teleseismic waves travelling through seismic and density models of the Earth to constrain the regional inversions. Application of this technique to dense gravity and seismic data arrays will allow us to illuminate structures of the lithosphere form below and obtain better images of the first 200kms depth geological structures. We aim at applying our adjoint theory-based inversion techniques on huge data sets collected during the PYROPE and TOPOIBERIA campaigns at the scale of the Pyrenees chain. In collaboration with BRGM and TOTAL companies through the "OROGEN" project we will perform full waveform inversion constrained by gravity data provided by BGI and BRGM to obtain both seismic velocities and densities. Pyrennees are a nice pilot site to validate our tools and we aim at applying them to other parts of the world like Western Australia and off-shore high resolution sites for which we already have huge oil company data. Joint gravity and seismic data are done recently in the Mauleon basin through pyrenees and will be improved in 2019 by introducing petrophysical and geological constraints in the same way that it is done for Mansfield and Yerrida region in Western Australia for gravity and magnetic data. The main goals of this joint inversion project are : (i)performing joint gravity and seismic inversions on PYROPE+BGI+TOTAL/OROGEN data sets using the adjoint method for the full sesismic waveform inversion in the Pyrénees (three south-North PRYROPE transects + Maupassacq) experiment) and introduce both petrophysical and geological constraints from the BRGM database (ii) performing joint inversion of gravity and teleseismic data collected on dense data arrays : SEAM II synthetic data and real Long beach/Los Angeles data (iii) applying the

methodology to other sites in the world : Western Australia (Yilgarn, Mansfield/Yerrida, Kimberley regions). (iv) applying the seismic data inversion tools to off-shore oil comapny data on multi-GPUs.

Dernières publications:

- J Giraud, V Ogarko, M Lindsay, E Pakyuz-Charrier, M Jessell, R Martin. Sensitivity of constrained joint inversions to geological and petrophysical input data uncertainties with posterior geological analysis.Geophysical Journal International 218 (1), 666-688 -
- G Dufréchou, R Martin, S Bonvalot, S Bruinsma. Insight on the western Mediterranean crustal structure from GOCE satellite gravity data. Journal of Geodynamics 124, 67-78. -

Caractérisation de milieux poreux par modélisation numérique multi-échelle de la propagation d'onde et d'écoulements (in)compressibles

Projet démarré en 2011

GET - Géosciences Environnement Toulouse (UMR 5563)

Porteur de projet: **Roland Martin**

In order to realise this project, we need 400 000 computation hours on pure CPUs OLYMPE and 6000 h of CPUS+GPUs (equivalent to 206 000 CPU hours). With this project we want to develop a numerical code Unisolver that allows us to image complex media with different rheologies like in granular and/or porous media in presence or not of fluids or attenuation. At different scales (micro to macroscale), interactions between fluids and solids must be taken into account in the wave propagation modelling. And for each phase intrinsic attenuation due to viscous or interphase friction effects must be taken into account. We model two different problems, one at the laboratory scale in granular or porous media and another one at the near surface scale. These models introduce similar mechanical behaviors : fluid-solid coupling, attenuation due to presence of fluids, etc... Different numerical techniques (high order finite differences, finite volumes or spectral elements) are used to model wave propagation in complex media at different scales. At the laboratory scale, porous media properties like permeabilities can be we evaluated at the Darcy or Biot scale to constrain our porous media models. We intend to develop here numerical tools to invert jointly seismic and electrical data to reduce model uncertainties at the near surface scale and to allow 4D monitoring of water resources. This project is a multidisciplinary project. AT GET laboratory, expertise is brought for wave propagation modelling using finite differences, finite spectral element methods and inversion tools are provided. At METIS laboratory, the data sets at the laboratory scale and the signal processing tools are provided. And at LAUM laboratory of Le Mans, V. Tournat provides physical expertise in granular and complex solid media in presence of water or not. With LAAS/Toulouse, the codes will be optimised with GET researchers on multi-CPU/multi-GPUs platforms.

Dernières publications:

- Quentin Brissaud, Roland Martin, Raphaël F. Garcia and Dimitri Komatitsch, Hybrid Galerkin numerical modeling of elastodynamics and compressible Navier-Stokes coupling: applications to seismo-gravito acoustic waves, Geophysical Journal International, vol. 210(2), p. 1047-1069, doi: 10.1093/gji/ggx185 (2017) -
- R. Martin , L . Bodet, V. Tournat, F. Rejiba. 3D numerical modelling of non-linear viscoelastic wave propagation using auxiliary differential equations. Geophysical Journal International, Volume 216, Issue 1, 1, 2019, Pages 453–469, https://doi.org/10.1093/gji/ggy441 - **doi:** pu.doi

Dynamique dans l'océan Atlantique Tropical et upwelling du Benguela

Projet démarré en 2011

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Isabelle Dadou**

A serious consequence of global warming that is increasingly gaining importance is the decrease of the dissolved oxygen content of the world ocean. Deoxygenation and extension of the oxygen minimum zones, in particular in the Eastern Boundary Upwelling systems, are predicted because oxygen is less soluble in warmer waters and also because the changing oceanic stratification and circulation are expected to reduce the supply of O2 to the ocean interior. However, the biogeochemical contribution due to the O2 consumed by the aerobic processes (e.g. remineralisation/respiration, nitrification) remains to be quantified. This deoxygenation of subsurface waters will have widespread consequences due to the role O2 and organic matter degradation plays in the biogeochemical cycling of carbon, nitrogen and other important elements such as P, Fe, Mn, S. Oxygen is essential to all aerobic life and sublethal and lethal O2 thresholds vary greatly between marine organisms. The oxygen minimum zones and associated upwelling regions are key areas where climatically relevant gases such as CO2, N2O, are released from the ocean to the atmosphere. In this area, the coupled physical/biogeochemical processes are very active, especially at (sub)mesoscale. In order to develop innovative predictive management tools and strategies to resolve the dynamic interactions of climate change drivers, i.e. changes in ocean circulation, climate, ocean acidification, etc. on the structure and functioning of marine ecosystems in these vulnerable oceanic areas, we propose to employ a combination of data synthesis and numerical simulations (coupled physical(ROMS)/biogeochemical(BioEBUS) model). We focus our efforts in the Tropical Atlantic ocean including the Benguela upwelling systems. During the year 2019, we will carry out different coupled physical/biogeochemical (ROMS/BioEBUS) simulations in the Tropical Atlantic Ocean including the Benguela upwelling system for the Alti-ETAO project (OSTST-CNES) (2017-2020).

Dernières publications:

- Bachèlery, M.–L., S. Illig, and I. Dadou, 2015, Interannual variability in the South–East Atlantic Ocean, focusing on the Benguela Upwelling System: Remote versus local forcing, J. Geophys. Res. Oceans, 121(1), 284–310. doi:10.1002/2015JC011168 - **doi:** pu.doi
- Bachèlery, M.–L., S. Illig, and I. Dadou, 2016, Forcings of nutrient, oxygen, and primary production interannual variability in the southeast Atlantic Ocean, Geophys. Res. Lett., 43, doi:10.1002/2016GL070288 - **doi:** pu.doi

Modélisation et assimilation de données pour l'étude de la circulation océanique dans le Golfe de Gascogne et autres régions côtières

Projet démarré en 2011

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Nadia Ayoub**

We aim at constraining a coastal OGCM with sea surface height and temperature satellite data. The objective is to provide a more realistic ocean state estimation at monthly time scales, with a specific focus on the surface layers. Modeling and assimilation in coastal areas present specific challenges because of the numerous physical processes that need to be taken into account and the wide range of their associated spatial and temporal scales. In such a context, data assimilation can effectively constrain the model if the method is able to take into account the complexity of the model error space due to the richness of the processes at work and to the specificity of the studied region. For this reason, we are working on an Ensemble Kalman Filter (EnKF) method where the full multivariate forecast error covariances are used. Our OGCM is SYMPHONIE in realistic configurations of the Bay of Biscay, North Western Mediterranean and Gulf of Tonkin. The ensembles are generated by randomly perturbing the wind forcing. We use the S-DAP (SEQUOIA data assimilation Platform) software that includes a code for the EnKF (http://sourceforge.net/projects/sequoia-dap/). From Dec 2018, we will start working on the circulation in the Gulf of Tonkin (Southern China Sea); we will perform ensemble simulations to quantify the model uncertainties

and explore the physical processes involved. We will focus on the variability of the Red River plume and its interactions with tides and wind-induced circulation over the shelf. Our objective for requesting computing resources at CALMIP is 1/ perform ensemble simulations and assimilation runs; these tests based on synthetic data allow us to evaluate the impact of both sea surface height and high-resolution sea surface temperature data on the estimation of the ocean surface circulation and stratification and calculate several types of ensemble statistics 2/ run the ocean model in a high resolution configuration (without assimilation) to study interactions between the river plume, tides and shelf circulation and to simulate altimetric observations of the future satellite mission SWOT, 3/ test the feasibility and performance of a downscaling method based on data assimilation in a high-resolution coastal model.

Dernières publications:

- Toublanc F., N. Ayoub, F. Lyard, P. Marsaleix, D. Allain, 2018. Tidal downscaling from the open ocean to the coast: a new approach applied to the Bay of Biscay. Ocean Modelling, 124, 16-32, doi: 10.1016/j.ocemod.201802001 - **doi:** pu.doi
- Ghantous M., N. Ayoub, P. De Mey-Frémaux, V. Vervatis, P. Marsaleix, 2020. Ensemble downscaling of a regional ocean model, Ocean Modelling, Vol. 145, doi: 10.1016/j.ocemod.2019.101511 - **doi:** pu.doi **url:** pu.open_url

Instabilités magnétiques dans les intérieurs stellaires

Projet démarré en 2011

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Laurène Jouve**

This proposal aims at understanding the interaction between differential rotation and magnetic fields in a stellar radiative zone. One possible application is the magnetism of main-sequence A-type stars, which possess a radiative envelope. Observations have revealed a lower bound in the strong magnetic field observed in a small fraction (5%) of those stars and a two orders of magnitude magnetic desert among those stars between this lower bound and a new type of sub-Gauss magnetism, first discovered in Vega. A bifurcation between stable and unstable large scale magnetic configurations in differentially rotating stars has been advanced to explain this apparent magnetic dichotomy. To test this scenario, we perform global 3D spherical simulations of a magnetic field subject to the differential rotation of a radiative stellar envelope, with the open-source MAGIC code. The first part of this project was devoted to the evolution of an incompressible magnetized fluid (Jouve et al, 2015). We then moved the project to a more realistic situation where stable stratification is taken into account. The time allocated in 2018 enabled us to finish the study of these stably stratified cases, initiated during the PhD of M. Gaurat. An article is in preparation on this subject. We then moved the project to the study of a forced differential rotation. D. Meduri, working as a postdoc in our group, performed a large parameteric study. Thanks to the calculations of session 2016 and 2017, he showed that when magnetic field is added, the flow is prone to MHD instabilities again. An article has been submitted on these subjects to Physical Review E. Hydrodynamical simulations performed by a Master student during the 1st semester of 2017 also enabled us to properly characterize the influence of the stable stratification and thermal diffusion on the calculated steady states, for values of the parameters realistic for stellar radiative zones. The hours allocated in 2018 enabled to start the study of the non-linear phases of possible MHD instabilities developing in such systems, in particular to investigate the possibility of dynamo action in stellar radiative zones. We wish to continue this study, both for the possibility of a dynamo action and for the transport of angular momentum induced by the instabilities. Finally, we are now interested in another type of forcing of the differential rotation, which consists in mimicking the contraction of a stellar radiative zone. This happens for example in red-giant stars for which asteroseismology provides us with information about the internal rotation rate. The main puzzle with those stars is that despite the contraction of their core and expansion of their envelope, the core is found to rotate 1 or 2 orders of magnitude slower than

what is expected from classical hydrodynamical models. Session 2018A enabled us to start the study of the axisymmetric hydrodynamical solutions produced by a contracting radiative zone. We now wish to continue those calculations by adding the effect of the stable stratification, density variation and later magnetic fields and studying the 3D stability of those solutions. The magnetic fields, especially if unstable, could indeed completely modify the redistribution of angular momentum in those astrophysical objects.

Dernières publications:

- Prat, V., Lignières, F., A&A, 566, 110, 2014 - **doi:** pu.doi
- Meduri, D., Lignières, F. & Jouve, L., PRE, 100, 013110 -

Mesure des vitesses horizontales de la surface solaire via la CST

Projet démarré en 2011

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Thierry Roudier**

Based on observations of the Sun, it seems clear that the medium which transfers the disturbances in the solar corona through the filament is the magnetic field. It is natural to study the evolution of the movement of material below the filament and the coronal magnetic field when specific motions can be imposed at the feet of the filaments. The goal of our program is to detect twisting or shearing of the filaments around the feet. Our first results show that the horizontal surface flows crossing the reversal polarity line where the filament is located, allow parasites polarities crossing the line inversion. Our studies also highlight the likely role of differential rotation for the destabilization of the filament, through the stretching of magnetic field lines, leading the filament to a sudden disappearance. The goal of our application to CALMIP is to measure the surface motions all over the Sun surface by using satellite images and Coherent Structure Tracking. The study of such large-scale photospheric motions is also a search on the precursors of solar flares and therefore contributes to the understanding of space weather.

Dernières publications:

- Link between trees of fragmenting granules and deep downflows in MHD simulation - **doi:** pu.doi **url:** pu.open_url
- Neural Network to Emulate Numerical Simulations of the Sun and Infer Synthetic Observations for Data Assimilation - **doi:** pu.doi

Modélisation océanique et atmosphèrique dans le Pacifique Sud-Est

Projet démarré en 2010

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Boris DEWITTE**

This project is the continuation of activities carried out within the project n°1044 focusing on modeling activities dedicated to the study of the Peru/Chile current system dynamics and the equatorial Pacific dynamics associated to extreme El Niño event. We plan to update our simulation based on updated oceanic Reanalyses (from Mercator) that serve as boundary conditions of our configurations, updated version of the code (in particular CROCO will replace our ROMS version) and taking into account new developments on air-sea coupling parametrizations. We also plan to start coupling a biogeochemical component to the existing platforms, which shall require tuning experiments and development. This project benefits from international collaborations and is in line with international projects within which the team is active (eg. TPOS2020, SCOR WG EBUS). A student has been

incorporated who will start using the models' configurations for their PhD works. The project benefits from support from two recently funded projects (ANR ARISE and SEPICAF funded by GMMC (Mercator)). Our needs for the first (second) semester of 2019 are estimated to 250000h (200000h), which is an amount comparable to the previous demand.

Dernières publications:

- Contreras M., O. Pizarro, B. Dewitte, A. Sepulveda and L. Renault, 2019: Subsurface mesoscale eddy generation in the ocean off central Chile. Journal of Geophysical Research. https://doi.org/10.1029/2018JC014723. - **doi:** pu.doi **url:** pu.open_url
- Garçon, V., Dewitte,B., Montes,I. and Goubanova, K., 2019, Land-Sea-Atmosphere interactions exacerbating ocean deoxygenation in Eastern Boundary Upwelling Systems (EBUS), in Ocean Deoxygenation:Everyone's problem, Causes, impacts, consequences and solutions, Eds D. Laffoley and J.M. Baxter, IUCN (International Union for Conservation of Nature and Natural Resources Report, Gland, Switzerland), pp 171-186. - **doi:** pu.doi **url:** pu.open_url

Calcul ab initio des propriétés de partage isotopique de minéraux et de solutions.

Projet démarré en 2010

GET - Géosciences Environnement Toulouse (UMR 5563)

Porteur de projet: **Merlin Méheut**

Measurement of the isotopic composition of minerals and rocks is a tool of primary importance to interpret geological processes. The last decade of geochemistry research has led to stable isotope measurements of unprecedented accuracy for many elements. In order to fully realize the full potential of these new measurements, it is important to understand the basic mechanisms causing isotopic fractionation through careful theoretical studies and laboratory experiments. Among the new elements that can be measured, silicon is of particular interest, both due to its ubiquity and high abundance in planetary environment (planetology and deep earth studies), and as an important nutrient for biosphere (environmental studies). Here we propose a systematic theoretical investigation of the equilibrium stable isotope geochemistry of silicon, supported by laboratory experiments and empirical studies of selected natural assemblages. Mineral-solution fractionation of Si will also be a focus of this investigation. While less abundant in Nature, Li isotopes show large isotopic fractionations between minerals and solutions, that have been recently investigated in details by experiments. They therefore represent a good case study of mineral-solution fractionation.

Dernières publications:

- Oxygen isotope fractionation during smithsonite formation from aqueous solutions - **doi:** pu.doi
- Pokrovski G. S., Kokh M. A., Proux O., Hazemann J-L., Bazarkina E., Testemale D., Escoda C., Boiron M-C., Blanchard M., Aigouy T., Gouy S., de Parseval P., Thibaut M. The nature and partitioning of invisible gold in the pyrite-fluid system. Ore Geology Reviews, 109, 545-563 -

Variabilité interannuelle de la circulation en Méditerranée occidentale

Projet démarré en 2009

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Claude Estournel**

The project aims at modelling the oceanic circulation in the whole Mediterranean basin at interannual scales with a focus on the Levantine basin where Levantine Intermediate Waters (LIW) are formed. Our projet is closely

associated to the PERLE experiment which takes place between october 2018 and 2020 with 3 cruises aiming at characterizig the formation and dispersion of the LIW. We are a partner of this project and our objective is to participate with our simulations from the preparation of the cruises to the scientific analysis of the results. All the studies listed above are associated to national and international projects (HYMEX and MERMEX) whose aim is to understand the modifications of the oceanic circulation and the consequences on marine ecosystems. The year 2019 is mainly devoted to improve the simulations which have been produced in 2018. The methodology will be based on sensitivity tests that will be done to find the origin of the bias in salinity that is currently noticed. The second part of the project are dedicated to the impact of extreme events in the coastal zone (AMORAD ANR project). The impact on sediment transport is now our objective with the coupling of SYMPHONIE and MUSTANG (IFREMER sediment model). The calibration of this model is in progress in the frame of the end of the PhD of G. Mikolajczak. Guillaume will continue as a post-doc to finalize his tudies and transpose them in the region of the Fukushima powerplant accident to assess the role of sediment on the transport of radionuclides.

Dernières publications:

- Damien P., Bosse A., Testor P., Marsalei P., Estournel C. Modeling post convective submesoscale coherent vortices in the Mediterranean Sea. Journal of Geophysical Research - **doi:** pu.doi
- Estournel C., Testor P., Damien P., D'Ortenzio F., Marsaleix P., Conan P., Kessouri F., Durrieu de Madron X., Coppola L., Lellouche J.M., Belamari S., Mortier L., Ulses C. and Prieur L. High resolution modelling of dense water formation in the north-western Mediterranean: benefits from an improved initial state in summer. Journal of Geophysical Research - **doi:** pu.doi

Peanuts

Projet démarré en 2009

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Francois Rincon**

Le processus d'accrétion de matière dans les environnements stellaires jeunes constitue une étape fondamentale de la formation des planètes. Il est désormais largement admis que la turbulence joue un rôle critique dans le processus d'accrétion, cependant la question de son origine au sein des disques reste encore en grande partie ouverte. Ce projet a donc pour objectif principal d'identifier et de mieux comprendre des mécanismes de transitions possibles vers la turbulence dans des écoulements en rotation différentielle Keplerienne représentatifs des systèmes accrétants. Nous utilisons pour cela des approches numériques originales dans le contexte astrophysiques mais utilisées dans d'autres communautés scientifiques. Il s'agit notamment de calculer des solutions non-linéaires 3D des équations pertinentes, dont on pense qu'elles représentent les briques fondamentales de la transition vers le chaos et la turbulence, et d'analyser de manière détaillée l'anisotropie des transferts spectraux non-linéaires dans le system Keplerien.

Dernières publications:

- "Periodic magnetorotational dynamo action as a prototype of nonlinear magnetic field generation in shear flows", J. Herault, F. Rincon, C. Cossu, G. Lesur, G. I. Ogilvie, P.Y. Longaretti, Phys. Rev. E 84, 036321 (2011) - **doi:** pu.doi **url:** pu.open_url
- "Magnetorotational dynamo chimeras. The missing link to turbulent accretion disk dynamo models ?", A. Riols, F. Rincon, C. Cossu, G. Lesur, G. I. Ogilvie, P.-Y. Longaretti, Astron. Astrophys. in press (2016) - **doi:** pu.doi **url:** pu.open_url

Astérosismologie des étoiles variables pulsantes

Projet démarré en 2002

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Stéphane Charpinet**

Evolved compact stars populating the extreme horizontal branch (also called sdB stars) and the white dwarf cooling sequence represent respectively an intermediate stage and the ultimate product of the evolution of intermediate to low-mass stars forming up to 98% of all stars in the Universe. The discovery of several classes of nonradial pulsators among these objects over the past decades has open huge opportunities to probe their interior with asteroseismology. These stars show rapid multiperiodic oscillations of low amplitude that are usually captured through high precision high speed photometry carried out from ground based mono- or multi-site campaigns, or from space instruments such as COROT, KEPLER, K2, and now TESS. These stars often show sufficient number of independent oscillation modes to allow in-depth probing of their internal structure and dynamic through asteroseismology. We have developed in our team powerful and unique numerical tools to exploit the asteroseismic potential of these stars. These include a massively parallel real-coded-hybrid-genetic-algorithm named LUCY that can perform high dimension multimodal optimization to "invert" the internal structure of these stars from the observed pulsation periods. This code, with appropriate stellar modeling and pulsation codes, is exploited and continuously improved with the goal to analyze objects among a still growing sample containing to date more than 110 known pulsating sdB stars and up to 200 pulsating white dwarfs, many of them having ultra high precision seismic data available from space instruments. This fantastic pool of seismic information about the interior of evolved stars requires important computational power to be fully exploited. Running our codes on CALMIP High Performance Computers has been the most efficient solution found so far to pursue this project.

Dernières publications:

- Charpinet, S.; Brassard, P.; Giammichele, N.; Fontaine, G., A&A, 628, L2 - **doi:** pu.doi
- Van Grootel, Valerie; Randall, Suzanna K.; Latour, Marilyn; Németh, Peter; Fontaine, Gilles; Brassard, Pierre; Charpinet, Stephane; Green, Elizabeth M. in Proc. of the PHOST conference - **url:** pu.open_url

Dans le cadre de la tache de service MESONH labélisé INSU Portage/Développement de modèle MésoNH sur architecture HPC

Projet démarré en 2001

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Juan Escobar**

MESO-NH Modélisation à moyenne échelle de l'atmosphère En 1993, des équipes de modélisation atmosphérique de méso-échelle du CNRM (Météo-France) et du Laboratoire d'Aérologie (UMR 5560) se sont regroupées au sein du projet MESO-NH visant à développer un nouveau code de modélisation météorologique intégrant les avancées scientifiques et techniques les plus récentes dans le domaine. Dès 1998, le projet a atteint ses objectifs initiaux et a débouché sur un outil de recherche performant du niveau des meilleurs codes de la communauté internationale. Il est aujourd'hui utilisé par une large communauté (atmosphériciens, hydrologues,...) de plus d'une centaine de chercheurs rattachés à 37 équipes dans 8 pays. Ce code : * intègre un système d'équations non-hydrostatique, permettant de traiter avec le même outil une vaste gamme de phénomènes atmosphériques allant de la méso-échelle alpha (quelques milliers de km) jusqu'à l'échelle des tourbillons (quelques m) * est doté d'un jeu complet de paramétrisations physiques, de divers niveaux de complexité et adaptées aux différentes échelles considérées * dispose de capacités d'auto-imbrication lui permettant de relever de nouveaux défis (prévisibilité des systèmes orageux par exemple) * est couplé avec des modules de chimie gazeuse, aqueuse et des aérosols qui offrent un cadre dynamique privilégié pour toute étude numérique de physico-chimie atmosphérique * est doté d'opérateurs d'observation qui permettent de comparer directement les sorties du modèle avec des observations

satellite ou radar. Les utilisations scientifiques de MESO-NH sont extrêmement variées. Le modèle est largement utilisé sur les thématiques des grands projets nationaux et internationaux (TOGACOARE, FASTEX, ACE II, TRACAS, PICO3, ESCOMPTE, ESQUIF, TRACE P, PEM, MAP, TROCCINOX, AMMA, MEDEX,...). L'INSU a labellisé les missions de Service (maintenance du code, assistance aux utilisateurs, veille scientifique)

Modes propres des étoiles

Projet démarré en 2001

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Michel Rieutord**

This project is devoted to various studies of stellar oscillations in order to give theoretical background to the interpretation of data coming from the space missions CoRoT (CNES) and KEPLER (NASA). The project is divided into three parts: the first part is focused on the oscillations of rapidly rotating stars and aims at deciphering the dynamics of both acoustic and gravity modes. The second part is devoted to the influence of magnetic fields and aims at modeling the oscillation spectrum of the so-called roAp stars. The third and last part focuses on the case of tidally forced oscillations, which are important for the understanding of the dynamics of binary stars. All these parts require in a more or less important way, 2D models of rotating stars and thus part of the computing time is dedicated to run and test such models (computed with the ESTER code).

Dernières publications:

- Gagnier D., Rieutord M., Charbonnel C., Putigny B. and Espinosa Lara F. (2019), ``Critical angular velocity and anisotropic mass loss of rotating stars with radiation-driven winds", in Astron. Astrophys., vol. 625, A88 - **doi:** pu.doi
- Gagnier D., Rieutord M., Charbonnel C., Putigny B. and Espinosa Lara F. (2019), ``Evolution of rotation in rapidly rotating early-type stars during the main sequence with 2D models", in Astron. Astrophys., vol. 625, A89 - **doi:** pu.doi

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4.4 Physique théorique et moléculaire

Optimisation de la radiothérapie interne par méthode Monte-Carlo

Projet démarré en 2019

CRCT - CRCT UMR 1037 - Centre de Recherches en Cancérologie de Toulouse

Porteur de projet: **Maxime CHAUVIN**

Targeted RadioTherapy (TRT) is a cancer therapy based on the administration of selective radiolabelled vectors. Currently, administration is most often based on fixed activities, eventually modulated by patient mass or body surface area. This approach disregards pharmacokinetics variability from one patient to another, and does not benefit from the possibility to follow the fate of the radioactive vector specifically for each patient (quantitative scintigraphic imaging using Single Photon Emission Computed Tomography - SPECT). Our objective is to implement a paradigm shift from "radioactive chemotherapy" towards "systemic radiotherapy", where each patient benefits from a personalised treatment based on the irradiation delivered specifically (dosimetry), from radiopharmaceutical uptake and washout. With this aim, our team develops innovative dosimetric approaches at various scales (cell, tissue, patient) by quantifying radioactivity distributions (SPECT) in the patient at different time after administration, and modelling radiation transport to assess the irradiation delivered (absorbed dose) for various emitters (alpha, beta, Auger) used in TRT. For that purpose, we use GATE, a Monte Carlo platform dedicated to medical applications based on Geant4. Monte Carlo methods are considered the current reference for modeling radiation transport and radiation-induced energy deposition, but they necessitate very long

computations time as they simulate every track and interaction of particles. For now, computations are performed on our local cluster (340 cores) but this solution is no longer adapted to ongoing projects. Therefore our proposal aims at using Olympe in a context of targeted radionuclide therapy, specifically to simulate SPECT quantitative imaging (European project MRT Dosimetry) and to produce reference dosimetric data (OpenDose project).

Calcul de dose en Radiothérapie Externe par Méthode Monte-Carlo

Projet démarré en 2019

CRCT - CRCT UMR 1037 - Centre de Recherches en Cancérologie de Toulouse

Porteur de projet: **Luc SIMON**

Approximately 50% to 60% of all cancer patients will receive external radiation therapy (RT) during their course of illness. Computing the dose received by the patient during RT is fundamental to assess local control and toxicity of the treatment. Limits of classic clinical algorithms for dose calculation are known for complex cases (heterogeneity, small fields...). Monte-Carlo methods are considered as the reference for the medical use of ionizing radiation and Geant4/GATE is an open-source Monte-Carlo platform dedicated to medical use. A GATE Monte-Carlo model of a radiotherapy device (Varian, TrueBeam) is implemented in our team (CRCT). Using our model promising results were published. Validation of our GATE model was performed by measurement on homogenous and heterogeneous phantoms. Percentage depth dose curves (PDD) and lateral dose profiles (LDP) were compared with experimental measurement (using films or ion chamber). These measurements were compared to our GATE Monte Carlo and also to a classic commercial algorithms (AAA, eMC). The results of GATE were closer to the measured dose distribution than the clinical algorithms. However, using Monte-Carlo method, computation of dose in a patient anatomy (using CT scan) is time consuming to simple media (because of the high number of voxels with different densities). For now computation are performed on our cluster (25 iMacs) but the performances are very limited. A test project on Olympe (calmip id: T18012, october 2017) shows spectacular improvement of computation speed. This project proposes to use Olympe for a study on 100 RT patients to perform an accurate dose computation for all types of treatments (SBRT, VMAT, photons, electrons, breast, lung, brain...). This would help medical physicists and physicians to have a better knowledge of the dose distribution in complex cases and to highlight the limits of clinical tools.

Roulage en milligravité : faisabilité et performance d'un rover à la surface d'un petit corps

Projet démarré en 2019

ISAE/DEOS - Département Electronique, optronique et signal

Porteur de projet: **Naomi Murdoch**

During the past decade, scientific interest in asteroids, comets, and small moons has led to an increase in the number of fly-by and in-situ missions to small bodies. This year alone holds two asteroid sample return missions. Hayabusa2, operated by the Japanese Space Agency, JAXA, deployed three hopping rovers to the surface of Ryugu between September and October, and plans to set down a fourth by July of 2019. NASA's OSIRIS-REx spacecraft will rendezvous with the carbonaceous asteroid Bennu in December, and will begin mapping its surface for potential sampling sites shortly after. Missions like those mentioned above will provide much needed insight into asteroid surface and chemical composition. However, the sheer number and diversity of small bodies within our observational range means that there remains much to be explored. Modeling and simulation provides a low-cost method to expand our knowledge of small body environments. For example, modeling regolith behavior at the grain scale can shed light on asteroid formation and morphology. This information is also critical for the design and operation of future in-situ small-body missions. At a high level, the purpose of this project is to study regolith behavior in micro-gravity conditions in order to augment our understanding of small body surface mechanics. This

analysis will be performed by using an open-source multi-physics dynamics platform to simulate granular flow around the wheels of a rover as it traverses the surface of Phobos, a moon of Mars.

Optique singulière dans les cristaux liquides

Projet démarré en 2019

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **gonzague agez**

Beam shaping is a basic need of photonic technologies (e.g., optical imaging, optical information and communication, optical manipulation, and laser processing of materials) and nowadays there are many techniques to control at will the spatial distribution of intensity, phase, and polarization. In general, this involves the use of optical elements that are designed to operate efficiently for a given wavelength, while user-friendly devices or some applications preferably require large spectral bandwidth. The goal of this project is to perform engineering of photonic structures based on the cholesteric liquid crystal phase. This soft material is inhomogeneous in the 3 dimensions and locally anisotropic. First, we will need to numerically generate a complex 3D periodic structure that mimics the real structure observed by electronic microscopy. Then, the beam shaping behavior will be simulated via FDTD (Finite Difference Time Domain) simulations. In these numerical analysis, the electromagnetic field propagation is solved through the designed material.

deep learning for nanophotonics

Projet démarré en 2019

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)
Porteur de projet: **Peter Wiecha**
During the last decade, great progress has been made in the field of artificial neural networks (ANNs) - computational models inspired by the human brain. ANNs are very efficient in analyzing large data-sets and they can be trained to categorize problems which are very hard to approach by traditional computational techniques. In this project we apply machine learning to remove barriers in the experimental and computational development of photonic nanostructures and metasurfaces. The research will explore training of ANNs to predict, accurately and in real-time, the far-field and near-field characteristics of individual nanostructures and complex collective arrangements. Such an approach will open up completely new paradigms in nano-optics and we will specifically address, new ideas for sub-wavelength information encoding and addressing of inverse problems. The project implies naturally the development of numerical methods and codes for electrodynamical simulations at a nano-meter scale. Those codes will be tested on CALMIP HPC and applied to open challenges in nano-optics research, such as multi-scattering in composed dielectric nanostructures or non-linear optical effects in the subwavelength regime. The developed tools will be also used to generate training data for artificial neural networks which will be trained on the HPC (preferably using the Nvidia V100 accelerator GPUs). Artificial neural networks will also be trained on experimental data. At the end of the year I will ask for a project for 2020A, where, in February 2020, I will start on a permanent position as chercheur at LAAS/CNRS.

Non-adiabatic dynamics and dissipation in the reactivity of PAH-related complexes and of molecule-surface systems

Projet démarré en 2018

LCAR - Laboratoire Collisions Agrégats Réactivité (UMR 5589)

Porteur de projet: **Didier Lemoine**

The present project seeks HPC support for two selected scientific projects. I. The ITN EUROPAH LCAR project aims at developing and applying new, efficient approaches to non-adiabatic dynamics and dissipation in the reactivity of PAH-related complexes. Namely, these approaches are built upon the Density Functional-based Tight Binding "DFTB" theory and upon its so-called Time-Dependent "TD-DFTB" version. Implemented in 2018 in the Toulouse open source DeMonNano package: a) TD-DFTB calculation of excited states, of their gradients and of the non-adiabatic (dynamical) couplings; b) Interfacing with a multiple-state mixed quantum-classical molecular dynamics scheme such as Trajectory Surface Hopping. For 2019 we plan in collaboration of the experimental group of Frank Lépile in Lyon: Applications to the relaxation of an electronically-excited PAH molecule; Analysis of direct versus indirect fragmentation and of the role of electronic-to-electronic and electronic-to-vibration energy conversions. II. The NEXT project addresses one key topic of EXcited STate dynamics At Surfaces: Adsorbate coupling to electron-hole pairs (EHPs) in reacting systems: Surface and subsurface chemistry of atomic and molecular hydrogen with Ag. The model systems are chosen to provide insights about how the elementary degrees of freedom of atoms or molecules (electronic, translational, vibrational and rotational) interact with EHPs. As an alternative to the TD-DFTB/TSH interface, the development of a friction version of molecular dynamics within DFTB-DeMonNano in 2018, extends computational feasibility to (much) larger systems and enables closer compararisons with experimental observations. For 2019 we plan: Full dimensional modeling of the collisions of gas phase and subsurface H atoms with silver surface and bulk atoms and with H adsorbates, including recombination reactions with the latter and for different isotopic combinations.

Dernières publications:

- Evgeny Posenitskiy, Mathias Rapacioli, Bruno Lepetit, Didier Lemoine and Fernand Spiegelman, Non-adiabatic molecular dynamics investigation of the size dependence of the electronic relaxation in polyacenes, Phys. Chem. Chem. Phys., 2019, 21, 12139 - **doi:** pu.doi

Physique des solitons dans les plasmas magnétisés

Projet démarré en 2018

LAPLACE - Laboratoire Plasma et Conversion d'Energie (UMR 5213)

Porteur de projet: **Renaud Gueroult**

Solitons are non-linear waves which feature unique properties. For example, solitons maintain their form while propagating in a dispersive media and also preserve their shape and speed after colliding with another soliton. Further to these unique physical properties, the concept of solitons has played a central role on theoretical developments in nonlinear wave physics and applied mathematics. We have shown through particle-in-cell simulations that shocks in magnetized plasmas can lead to the formation of magnetosonic solitons, both in perpendicular astrophysical shocks [1] and in fast magnetic compression experiments [2]. We have also recently shown using the same tools that solitons exhibit peculiar properties when propagating to a plasma/vacuum interface [3]. One of the long standing questions in astrophysics is what acceleration mechanism can explain the observation of cosmic energetic particles. Here, the new result that solitons can under some conditions mediate the reformation process [1] by which astrophysical shocks propagate offers new avenues to study particle shock acceleration and its role on energetic particles. Furthermore, improving our basic understanding of the physics of solitons in magnetized plasmas could also help designing control techniques to mitigate the effects of electron dephasing which typically limit the performances of plasma-based particle accelerators [2]. Finally, solitons may find applications for plasma control owing to the plasma displacement they can produce [3]. We propose here to build on our earlier results from Refs [1,2,3] and to explore and study the rich physics uncovered by these past studies using electromagnetic particle-in-cell (PIC) simulations. [1] Gueroult R., Ohsawa Y. and Fisch N.J, Physical Review Letters, 118, 125101 (2017) [2] Gueroult R., Fisch N. J., Physics of Plasmas, 23, 032113 (2016) [3] Gueroult R., Fruchtman, A. and Fisch, N. J., Physics of Plasmas, 25, 062118 (2018)

Dynamique microscopique d'agrégats ou de molécules sous irradiation intense

Projet démarré en 2012

LPT - Laboratoire de Physique Théorique (UMR 5152)

Porteur de projet: **Phuong Mai Dinh**

The structure and the dynamics of a collection of atoms (molecules, clusters, nanostructures, materials, etc.) come from a subtle balance between electronic effects (by essentially valence electrons) and ionic ones (an ion being the remaining system composed by the atomic nucleus and the core electrons). The analysis of the dynamics of such objects relies on a simultaneous description of the electronic and ionic degrees of freedom. The difference between the femtosecond time scale of (quantum) electrons and that of the (classical) ions, of the order of the picosecond, makes this task difficult. To simulate realistic processes with many electrons/ions, a goal that represents a real theoretical and numerical challenge, we have developed tools to cope this multiscale dynamics, from the femtosecond to the picosecond. Relying on our expertise of more twenty years on the ionization of free clusters by intense electromagnetic excitations, this project aims at studying dynamical scenarios when a molecule or a cluster is irradiated by a laser. In particular, the advent of new sophisticated light sources, as train of attosecond pulses in the XUV, opens the road for new types of excitation and ionization in multielectronic systems. At the same time, the use of higher and higher laser intensities calls for a better description of dissipation in such systems, and therefore calls for "beyond mean-field" approaches. Finally, we would like to extend our approach to the case of irradiation of small systems by an electron or a positron, this project being motivated by a brand-new collaboration with an experimentalist and a theoretician in Lyon and financially supported by ANR.

Dernières publications:

- L. Lacombe, P.-G. Reinhard, E. Suraud, and P. M. Dinh, Annals of Physics, 406 (2019) 233 - **doi:** pu.doi
- T. Brabec, P.M. Dinh, C.-Z. Gao, C. McDonald, P.-G. Reinhard, and E. Suraud, Physical mechanisms encoded in photoionization yield from IR+XUV setups - **doi:** pu.doi

Plasmonique hybride

Projet démarré en 2011

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Christian Girard**

This project aims to get a better understanding of optical properties of plasmonic structures composed of colloidal and lithographied metal nanoparticles deposited on dielectric substrates and their coupling with fluorescent nanoparticles. The team has already a solid experience in that field, theoretically as well as experimentally (see references for more information). A program based on Green's dyadic method has been developed. This algorithm reproduces with a good agreement experimental results, but it needs an efficient supercomputer such as EOS and now Olympe, to be run in reasonable times. In that perspective, we are parallelizing our programs. It will allow us to study more complex structures with a better precision.

Dernières publications:

- Applied optics 58 (7), 1682-1690 (2019) -
- Advanced Optical Materials, 1801787 (2019) -

Agrégats quantiques

Projet démarré en 2010

LCAR - Laboratoire Collisions Agrégats Réactivité (UMR 5589)

Porteur de projet: **Nadine Halberstadt**

In this project we study dynamics processes in or on quantum clusters. We focus on helium droplets, which exhibit outstanding superfluid properties. The challenge consists in describing the N-body dynamics as a function of time and taking into account the quantum nature of helium. We are also making extensive use of the simulation program of Barranco and Pi, from the Barcelona University, which is based on helium density functional (He-DFT) and its time-dependent version. We will use it to describe the clustering of atoms and the photodissociation or dissociative photoionization of molecules or cluster in helium nanodroplets. We will also take advantage of the IDEX Chaire d'Excellence of Manuel Barranco to start developping a mixed approach with the MCTDH techniques for the dopant and their nearest neighbor helium atoms, and He-DFT for the rest of the droplet. With W. Unn Toc and Ch. Meier we have developped a simulation method based on MCTDH (Multi-Channel Time-Dependent Hartree) in Gaussian wave packets (GWP), to take into account both correlation and boson exchange symmetry. The first approximation of this method, ZPAD (zero-point averaged dynamics), will be tested in comparison witht he He-TDDFT results in order to determine the important parameters for MCTDH using GWP.

Dernières publications:

- Fall-back time for photo-ionized Cs atoms attached to superfluid 4He nanodroplets, F. Coppens, J. von Vangerow, A. Leal, M. Barranco, N. Halberstadt, M. Mudrich, M. Pi, and F. Stienkemeier, Eur. Phys. J. D 73, 94 (2019); - **doi:** pu.doi
- Dynamics of impurity clustering in superfluid 4He nanodroplets, F. Coppens, F. Ancilotto, M. Barranco, N. Halberstadt, and M. Pi, Phys. Chem. Chem. Phys.21, 17423 (2019); - **doi:** pu.doi

Simulation numérique des propriétés optiques de nano-objets et de métasurfaces optiques

Projet démarré en 2008

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Arnaud Arbouet**

This project aims at predicting the optical properties of metallic or semiconducting nanostructures as well as optical metasurfaces composed of several of these nano-objects. It is well-known that gold and silver nanostructures support optical resonances termed surface plasmon resonances, the properties of which strongly depend on the particle morphology, its size and environment. The ability of Surface Plasmons to enhance the electric field and shrink it into regions of subwavelength dimensions open exciting perspectives in nano-optics. The investigation of the peculiar properties of Surface Plasmons has motivated several important experimental breakthroughs such as near-field optical probes, electron spectroscopies and nonlinear microscopies. The modelization of these complex experiments is the main motivation of the present project. The interpretation of nano-optics experiments requires the resolution of Maxwell's equations taking into account the morphology and material properties of a given nanosystem. In our case, we use the Green Dyadic Method and use a discretization of the volume of the investigated nanosystems. This has clear advantages as virtually particles of any shape can be described but it also has important constraints as the size of the linear systems to be manipulated in our algorithms can be quite large. The numerical implementation of our resolution algorithm is based on an hybrid OpenMP/MPI parallelization which fully exploits the ressources of EOS.

Dernières publications:

- P. R. Wiecha, C. Majorel, C. Girard, A. Arbouet, B. Masenelli, O. Boisron, A. Lecestre, G. Larrieu, A. Cuche, V. Paillard, Tailoring electric and magnetic dipole emissions by high-refractive index dielectric nanostructures. META 2019, Symp. I "Hybrid photonic and plasmonic materails for sensing, energy conversion and imaging applications", Lisbon, Portugal, July 24-27, 2019. Invited Talk - **doi:** pu.doi

- High brightness ultrafast transmission electron microscope based on a laser-driven cold-field emission source: principle and applications. Advances in Physics: X, 4, 1660214 -

Molécules sur surface

Projet démarré en 2008

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Xavier Bouju**

Our studies on the adsorption of molecules on metal surfaces will continue in 2018. We plan to address relatively large molecules in terms of size which will require significant calculations. Right now, we plan to use semi-empirical methods, although the use of DFT can also be considered. The metal surfaces we expect to use are surfaces conventionally used as Au (111). We are considering the possibility to tackle the adsorption of molecules near surface defects, such as kinks or step edges.

Dernières publications:

- Giant (12×12) and (4×8) reconstructions of the 6H-SiC(0001) surface obtained by progressive enrichment in Si atoms - **doi:** pu.doi
- Three-dimensional hydrogen bonding between Landers and planar molecules facilitated by electrostatic interactions with Ni adatoms - **doi:** pu.doi

Simulations quantiques des processus ultrarapides dans des systèmes complexes

Projet démarré en 2002

LCAR - Laboratoire Collisions Agrégats Réactivité (UMR 5589)

Porteur de projet: **Christoph Meier**

The aim of the project «Simulations quantiques des processus ultrarapides dans des systèmes complexes» is the theoretical study and numerical simulation of atomic and molecular processes at the femtosecond timescale. In particular, the quantum aspects of the time evolution, and the possibility to actively control its dynamics by shaped laser pulses are at the hart of the project. In many areas, quantum effects are extremely important for the detailed understanding of the dynamical processes at the atomistic level, like chemical reactivity, catalysis or biological functioning. Additionally, quantum dynamics in general, its coupling to an environment and the possibility to control its time evolution are keystones for possible future implementations of quantum information processing. As far as the possibility to control quantum processes are concerned, several experimental advances have substantially increased the general interest , like pulse shaping techniques, developed in the optical regime,that have been transposed to : -- the UV/XUV regime, with a possibility to control the optical phase withing the intensity of the envelope (carrier / envelope phase), opening new possibilities for attosecond control of atomic processes. -- the IR regime, with the possibilty to control nuclear dynamics directly on the electronic ground state From the theoretical point of view, the dynamic quantum mechanical modelling of atomic processes are still restricted to a few degrees of freedom, very often insufficient for complex systems, like proteins, or embedded or deposited molecules and clusters. In this context, the complexity not only stems form the number of atoms involved, but also from the from the different types of interactions, the effects of a coupling to an environment, and the non-linear response to strong, external pulses of high complexity. As a consequence, the development of novel quantum or mixed quantum/classical methods is an important part of the project, alongside with simulations of realistic systems with well established methods.

Dernières publications:

- "Quantum dynamics modeled by interacting trajectories" L. Cruz-Rodriguez, L. Uranga-Pina, A. Martinez-Mesa, and C. Meier, Chem. Phys. 503, 39 (2018) -
- Quantum trajectory study of laser-driven atomic ionization, L. Cruz-Rodriguez, L. Uranga-Pina, A. Martinez-Mesa, and C. Meier, Chem. Phys. 715, 211 (2019) -

APPLICATIONS DES METHODES DU CHAOS QUANTIQUE: INFORMATION QUANTIQUE, PHYSIQUE DU SOLIDE, PHYSIQUE ATOMIQUE, ETUDE DES RESEAUX

Projet démarré en 2001

LPT - Laboratoire de Physique Théorique (UMR 5152)

Porteur de projet: **Bertrand Georgeot**

The project is devoted to the application of methods from quantum chaos to solid state physics, quantum computation, atomic physics and networks. A first part of the project studies studies the effects of interaction on many-body systems, in particular the transition towards a quantum chaos regime characterised by delocalized wavefunctions. This theme was originally developped in the context of the Anderson localization of electrons in solids, which is still studied in the group in particular in the understanding of the multifractal properties of the wave functions at the transition. A second aspect of the project concerns the simulation of chaotic systems by a quantum computer. Algorithms developped in the group, enabling to simulate efficiently quantum and classical physical systems in a regime of dynamical chaos, are implemented and tested in presence of realistic imperfections. These developments towards the study of quantum computers led us to more fundamental studies on decoherence in quantum systems, the creation of entanglement and interference in quantum processes, and their link with the efficiency of quantum algorithms. A recent development concerns the study of molecular computation in link with experimentalists at CEMES. These studies and the recent experimental progress in the control of cold atoms led us to new developments towards the application of these different methods to the physics of cold atoms and Bose-Einstein condensates. A new direction recently initiated corresponds to the application of these methods to networks like the World Wide Web, in particular in the context of the Google PageRank algorithm.

Dernières publications:

- K.M.Frahm and D.L.Shepelyansky, "Google matrix analysis of bi-functional SIGNOR network of protein-protein interactions", submitted to Bioinformatics Oxford 28 August (2019) arxiv:1909.10975 -
- M.Y.Zakharov, D.Demidov and D.L.Shepelyansky, "Thermoelectric properties of Wigner crystal in two-dimensional periodic potential", submitted to Eur. Phys. J. B 28 Oct (2019) (arXiv:1910.12946) -

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4.5 Chimie quantique

Activation de petites molécules par des complexes métalliques

Projet démarré en 2019

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Laurent Maron**

Our team, within the LPCNO, focuses on modulation, investigation of molecular structures and/or interactions on an atomic level. The use of computational chemistry is increasingly being utilized and further understood; applicable to a variety of chemical problems. We are submitting a request for hours in order to continue our research and research collaborations. Analysis of the reactivity concerning S, D or F block elements provide insight into the durability and malleability of these complexes. Particularly, lanthanide chemistry is a point of interest.

This technique allows exploration of electron localization and therefore an insight into the possible mechanism(s) of interaction. Research is not limited to metallic complexes whereby collaboration worldwide allows our team to explore other problems such as activation of small molecules – an increasing area of interest. The activation of small molecules refers to the mechanism in which manipulation of an atomic bond – polarization for example – can infer possible kinetic control and/or the formation of a variety of novel products. Computational techniques exploit the understanding of the quantum nature of atoms and their subsequent interactions.

Processus collisionnels élémentaires dans les jets de plasma d'hélium dans l'air

Projet démarré en 2019

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Thierry Leininger**

The main objective of the present project is an in-depth understanding, both qualitative and quantitative, of elementary collision processes that lead to the formation of secondary ions when a plasma jet of helium is diluted in the air. In fact, a close collaboration between three laboratories (LCPQ, LAPLACE and IT4I) involved in this project, which began five years ago, has up now to provided extensive data on the processes taking place inside the plasma generator and the goal of the present project is to extent those studies to collisions occurring after the helium plasma jet leaves the generator and gets into contact with the surrounding environment (air). More specifically, the project represents a part of a broader research intention aimed at providing, from first principles, the data needed for a macroscopic modeling of plasma jets based on Navier-Stokes equations coupled to the Poisson and diffusion equations. These models will be used for the development and optimization of non-thermal helium plasma generators at atmospheric pressure.

Développement d'un modèle mixte de chimie quantique et d'apprentissage automatique pour prédire les paramètres RMN de structures de carbone amorphe

Projet démarré en 2019

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)

Porteur de projet: **Céline Merlet**

Porous carbons are an important class of materials used in many applications including energy storage, gas storage, water treatment, and catalysis. In all cases, the characterisation of these materials, still challenging from an experimental point of view, is an essential step in order to understand and optimise the performance of the systems. As a consequence, many theoretical works have aimed at generating atomistic structures which are very helpful to study structure-property relationships. Techniques used include Hybrid Reverse Monte Carlo and Quench Molecular Dynamics. While these models are extremely useful to get insights into the microscopic mechanisms of adsorption, it is hard to assess precisely the quality of these structures. This is due in part to the challenge of obtaining quantitative experimental data (e.g. proportions of 5-/6-/7-membered rings) and the ambiguity of some results (i.e. structures with different local structures and ring counts can have very similar pair distribution functions). Recently, Nuclear Magnetic Resonance has been investigated as a promising technique to improve our understanding of such structures. So far, the interpretation of NMR spectra of adsorbed molecules has mainly relied on the calculation of chemical shifts for small aromatic molecules (e.g. benzene, coronene). Nevertheless, the porous carbons used in common applications are extended solids, with defects, for which current models are not suitable. Our aim is to develop a combined quantum chemical / machine learning based model to predict NMR parameters in large amorphous carbon structures and use it to improve our understanding of such disordered solids. The approach will be based on coupling a tight-binding model with tunable atomistic magnetic polarisabilities. The model should then allow us to better understand the influence of defects on the

electronic and magnetic properties of the carbons as well as discriminating between various proposed atomistic models.

Modélisation de l'activation de liaisons chimiques inertes par des complexes organométalliques via un nouveau mode de coopération métal-ligand

Projet démarré en 2018

LCC - Laboratoire de Chimie de Coordination (UPR 8241)

Porteur de projet: **Dmitry Valyaev**

The proposal is focused on the theoretical study of the activation of inert E-H bonds (E = H, B, C, Si) by transition metal complexes using a new mode of metal-ligand cooperation. The project is based on the experimental results recently obtained in the team "Molecular design of transition metal pre-catalysts" of Laboratory of Coordination Chemistry (LCC), namely facile dihydrogen activation by a series of manganese complexes bearing bidentate ligands incorporating phosphine and N-heterocyclic carbene moieties and their high activity in hydrogenation of carbonyl compounds. The first part of the project will be devoted to the study of the electronic structure and bonding mode of the reactive manganese intermediates and the mechanism of E-H bond activation (concerted or stepwise). Then the modeling of entire catalytic cycle for selected manganese catalysts and relevant model organic substrates (ketones, imines, esters, alkynes) as well as the expansion of this concept to other first row transition metals (Fe, Co, Ni) will be performed.

Dernières publications:

- "Phosphine-NHC Manganese Hydrogenation Catalyst Exhibiting a Non-Classical Metal-Ligand Cooperative H2 Activation Mode", R. Buhaibeh, O. A. Filippov, A. Bruneau-Voisine, J. Willot, C. Duhayon, D. A. Valyaev, N. Lugan, Y. Canac, J.-B. Sortais, Angew. Chem. Int. Ed. 2019, 58, 6727–6731. - **doi:** pu.doi

Systematic study of the structure and bonding of halogens on low index Pt surfaces

Projet démarré en 2018

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Chiara Dinoi**

Heterogeneous catalysis is one of the most important chemical processes of various industries performed on catalyst nanoparticles with different sizes or/and shapes. In the past two decades, thanks to the spectacular advances in syntheses of metal nanomaterials, the catalytic performances of different catalytic reactions on metal nanoparticles with well controlled sizes or shapes have been extensively studied. It has been shown, in particular, that the structure and morphology (size and shape) of metal nanoparticles may have a substantial influence on their catalytic activity. One of the current goal of nanoscience and nanotechnology is therefore to provide the ability to create controlled structures and geometries to investigate and optimize a broad range of catalytic processes. The team of B. Chaudret and K. Soulantica recently discovered that the presence of different halides on the surface of Pt nanoparticles influences the growth mode of these particles, leading to different catalytic activities and selectivities during the catalytic hydrogenation process of several compounds. The synthesis of Pt nanoparticles, obtained by reaction of Pt halides with octadecylamine under exogenous H2 pressure, indeed, has shown that the use of PtCl2 at a 99.9% of purity affords Pt nanoparticles with a multipode crystallographic orientation, whereas the use of PtCl2 at a 98% of purity (containing therefore other halides as impurity) affords Pt nanoparticles with a concave cube crystallographic orientation in the 110 surface. Interestingly these two crystallographic orientations, either multipodes or concave cubes, display different catalytic activities and selectivities in the catalytic hydrogenation reaction of several substrates. To understand the reason for this

behavior, we recently started, in collaboration with this experimental group, a theoretical work aimed at studying the structure and bonding of halogens on Pt low index surfaces (100, 110 and 111) by means of density functional theory (DFT) calculations using periodic slabs to model the surface. By computing the halogen absorption energies, in particular, we plan to determine which halogens (or mixtures of halogens) are preferentially absorbed by a fixed surface and which surface has the lower absorption energy for a fixed halogen (or mixture of halogen). Once we have determined and explained the correlation between the halogen composition and the structure of the Pt nanoparticules, our second goal is to establish the correlation between the shape of the Pt nanoparticule surfaces and the corresponding catalytic performances.

Etude des propriétés photophysiques de complexes d'Iridium(III)

Projet démarré en 2018

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Fabienne Alary**

Cyclometalated iridium(III) complexes typically display intense and highly tunable luminescent emission and can be used as phosphors incorporated into light-emitting electrochemical cell devices for artificial lighting applications, as molecular sensors and as phosphorescent cellular imaging agents for confocal microscopy. Key to their exploitation in these applications is the engineering of the organic ligand supporting the metal centre to enable efficient tuning of the electronic and electrochemical properties. These ligand tuning effects can also determine the localisation and character of the emissive excited state which can have a profound influence on the photophysical properties. In the current project a series of cationic biscyclometalated iridium(III) complex incorporating a pyridyl- (pytz) , pyrimidinyl- (pmtz) or pyrazinyltriazole-based (pztz) ancillary ligand have been experimentally prepared and their photophysical properties investigated. The data show that the ancillary ligand has a significant affect on the photophysical properties leading to a general trend of increasing wavelength of emission in the order pytz < pmtz < pztz. Further, the change in the nature of the ancillary ligand leads wo a switching in the nature of the emissive state from 3MLCT/3ILCT character (MLCT = metal-to-ligand charge transfer, ILCT = intraligand charge transfer) favoured for pytz to 3MLCT/3LLCT for pztz based complexes (LLCT = ligand-to-ligand charge transfer). In addition, for some of the complexes the excited state is observed to switch between these states on warming from 77 K (3MLCT/3ILCT) to room temperature (3MLCT/3LLCT). Indeed, it is significant that for the complex [Ir(ppy)2(pmtz)]+ dual emission from both excited states persists to above room temperatures. The aim of this study, with experimental data directly comes from our collaborator Paul Elliott (U. Huddersfield, UK),is therefore to provide crucial computational data in in order to understand that photophysical properties of these complexes and offer insights into the emissive excited state dynamics involved. This will entail the optimisation of the ground state and lowest triplet excited states of each complexes, the calculations of their optical absorption spectra and characterisation of the transition involved, determination of the electronic structure through examination of their molecular orbitals and determination of the localisation of the emissive states.

Photoréactivité de complexes de ruthénium(II) et d'osmium(II)

Projet démarré en 2018

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Isabelle Dixon**

Ruthenium complexes are inescapable in solar energy conversion, photocatalysis or photodynamic therapy. They lie at the heart of novel anticancer therapeutic strategies involving the photorelease of biologically active moieties. Microscopic photoreactivity mechanisms have remained elusive during 40 years because they involve

excited states that bear no distinct spectroscopic signature (so-called 'dark states'). In 2016, for the first time, our theoretical calculations [a] have allowed us to identify and rationalize the key role of such excited states in photorelease mechanisms, opening the way to a better understanding of photoinstability issues in this family of complexes. This project aims at extending these studies to a large family of complexes (Ru/Os) that display rich and original photoreactivities. Experimental data directly comes from two of our collaborators (Paul Elliott, U. Huddersfield, UK [b] and Sylvestre Bonnet, U. Leiden, NL [c]), following interactive approaches combining experiment and theory in close synergy. [a] Göttle, A.J.; Alary, F.; Boggio-Pasqua, M.; Dixon, I.M.; Heully, J.-L.; Bahreman, A.; Askes, S.H.C.; Bonnet, S. Inorg. Chem. 2016, 55, 4448. [b] Welby, C. E.; Rice, C. R.; Elliott, P. I. P. Angew. Chem. Int. Ed. 2013, 52, 10826; Scattergood, P. A.; Ross, D. A. W.; Rice, C. R.; Elliott, P. I. P. Angew. Chem. Int. Ed. 2016, 55, 10697; Scattergood, P. A.; Khushnood, U.; Tariq, A.; Cooke, D. J.; Rice, C. R.; Elliott, P. I. P. Inorg. Chem. 2016, 55, 7787. [c] Cuello-Garibo, J.-A., Pérez-Gallent, E., van der Boon, L., Siegler, M. A., Bonnet, S., Inorg. Chem. 2017, 56, 4818.

Dernières publications:

- Theoretical Chemistry Accounts (2018) 137:37 - **doi:** pu.doi
- Inorg. Chem. 2018, 57, 3192−3196 - **doi:** pu.doi

Stochastic Quantum Chemistry

Projet démarré en 2018

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Pierre-François Loos**

In the last decade, supercomputers and their ever-growing capabilities have transformed the way one must think and implement quantum chemistry algorithms. In the footsteps of this technological shift, this project aims at revisiting the traditional quantum chemistry methods to make them stochastic by nature. Contrary to their conventional, deterministic parents, these methods are well suited to massively parallel architectures and have proven to be scalable up to hundreds of thousands of cores. A key aspect of this proposal is validate a number of strategies to make the stochastic implementation of these methods both general and practical for large systems. In particular, we propose to take advantage of the zero-variance principle in order to significantly reduce the statistical uncertainty and weds deterministic and stochastic algorithms to produce an hybrid semi-stochastic massively-parallel method, thereby achieving the best of the two worlds.

Dernières publications:

- A Mountaineering Strategy to Excited States: Highly-Accurate Reference Energies and Benchmarks Pierre-François Loos , Anthony Scemama , Aymeric Blondel , Yann Garniron , Michel Caffarel and Denis Jacquemin (2018), in: Journal of Chemical Theory and Computation, 14:8(4360-4379) - **doi:** pu.doi **url:** pu.open_url
- Selected configuration interaction dressed by perturbation Yann Garniron , Anthony Scemama , Emmanuel Giner , Michel Caffarel and Pierre-François Loos (2018), in: J. Chem. Phys., 149:6(064103) - **doi:** pu.doi **url:** pu.open_url

Mechanism of a Ru catalysed concomitant dihydrogen/B-H activation process: a computational study

Projet démarré en 2017

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Chiara Dinoi**

The use of transition metal catalysts may allow the challenging activation of unsaturated bonds such as the inert E-H σ-bonds (E= H, B, Si, C, N). Contrarily to the C=C bond engineering, the synthetic strategies relying on the formation and post-functionalization of embedded-Bsp2-Nsp2 bonds remain challenging and still under-explored. As pioneered by Dewar, they are mostly obtained by Friedel-Crafts cyclization reactions leading to conjugatively stabilized Bsp2-Nsp2 bonds such as azaborines and related compounds.Other approaches such as intramolecular hydroboration or dehydrogenative cylization have also been reported to a lesser extent for the synthesis of different BN-embedded molecular scaffolds. We investigate here the formation of Bsp2-Nsp2-embedded cyclic systems via a recently discovered Ru catalysed concomitant dihydrogen/B-H activation process. As attested by NMR and X-ray diffraction studies this catalytic reaction affords uncommon benzazaborolidines species in good yields. We plan here to study from a theoretical point of view the nature of this catalytic transformation by using DFT calculations. The thermodynamic aspects as well as the mechanistic profile of the reaction will be rationalized and the main parameters enabling the activation processes involved in this selective and efficient transformation will be investigated.

Dernières publications:

- Beguerie, M.; Dinoi, C.; del Rosal, I.; Faradji, C.; Alcaraz, J.; Vendier, L.; Sabo-Etienne, S., ACS Catal., 2018, 8, 939-948. -

Structuration de mélanges de semi-conducteurs organiques pour la photo détection. Etude sur les propriétés photophysiques et photochimiques.

Projet démarré en 2016

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Fabienne Alary**

This demand is a cooperative project between four public laboratories in Toulouse (LAAS, Laplace, LCC, LCPQ). Our main objective is to reach a detailed understanding of the electronic structure and of electronic transfers occurring at interfaces present in organic photovoltaic (OPV). Achieving this goal will able us to design and to synthetize original and efficient organic devices for photoconversion. The description of the nano-morphology created upon blending of the two organic semi-conductors (OSCs) will be the subject of extensive theoretical and experimental studies in order to achieve a rationalization and a full description of the electronic phenomena such as the efficiency of excitons diffusion as well as the efficiency of dissociation into free charges from which originates the current. The interfacial morphology and its electronic interactions will be studied by using a set of advanced characterization methods.

Dernières publications:

- JOURNAL OF PHYSICAL CHEMISTRY A. 122, 6532-6545. - **doi:** pu.doi

Etudes théoriques des espèces moléculaires impliquées dans les premiers instants de synthèse de nanoparticules métalliques

Projet démarré en 2016

LCC - Laboratoire de Chimie de Coordination (UPR 8241)

Porteur de projet: **Christine Lepetit**

The morphology and the size of the metallic nanoparticles (NPs) prepared in the team Nanochemistry Organisation and Sensors (NOS) in LCC, are strongly dependent of the organometallic precursor and synthesis route, which are determinant for the control of the microelectronic, plasmonic or biological applications of these nano-objects. In order to help in understanding and controlling the nano-objects nucleation and growth processes,

the organization of the metallic centers and the chemical reactivity of the molecular species formed during the very first steps of the organometallic synthesis, will be studied using various theoretical tools that will be calibrated from the available experimental spectroscopic data (X-Ray Diffraction, Nuclear Magnetic Resonance (NMR), Infrared (IR) and Raman spectroscopy). On the one hand, using a computational molecular approach, a series of mono- or polymetallic, homo- ou hetero-metallic precursors built with various metallic centers (M or M' = Ni, Cu, Zn, Ag) in various oxidation states and with various amidinate ligands substitution patterns, will be studied using ELF (Electron Localization Function) topological analysis, QTAIM (Quantum Theory of Atoms In Molecules) and NCI (Non-Covalent Interactions) analysis, in order to characterize metal-ligand bonding and metal-metal interactions. On the other hand, the interactions between the stabilizing ligand and the surface metal atoms of the metallic nanoparticle will be investigated using periodic DFT calculations and QTAIM and ELF topological analyses, and carried out for crystalline metallic surfaces used as models of the facets of the nanoparticles.

Dernières publications:

- Z. Zhao, Y. Coppel, J. Fitremann, P. Fau, C. Roux, C. Lepetit, P. Lecante, J.-D. Marty, C. Mingotaud, M. L. Kahn Mixing time between organometallic precursor and ligand: a key parameter controlling nanoparticle size and shape and processable hybrid materials. Chem. Mater. 2018, 30(24), 8959–8967 - **doi:** pu.doi
- R. Taakili, C. Lepetit, C. Duhayon, D. Valyaev, N. Lugan, Y. Canac, Palladium(II) pincer complexes of a C,C,C-NHC, diphosphonium bis(ylide) ligand.Dalton Trans. 2019, 48, 1709–1721. -

Dianions géminés: des complexes carbéniques aux complexes dimétalliques

Projet démarré en 2016

LHFA - Laboratoire d'Hétérochimie Fondamentale et Appliquées (UMR 5069)

Porteur de projet: **Marie Boutignon**

Due to the increasing number of examples of stable geminal dianions, this kind of species received a growing interest in the 2000's (ACIEE 1999, 38, 1483-1484). The double negative charge carried by a single carbon atom proved to be easily stabilized by a various set of electron-withdrawing substituents, from silyl groups to hypervalent phosphorus. This interest was also supported by the fact that such geminal dianions can be used as precursor for the synthesis of carbene complexes of various metals, especially d0 metals and rare earths metals (Chem. Soc. Rev. 2011, 40, 2164). In some case they also proved to act as non-innocent ligands for CH activation (Organometallics 2005, 24, 4838-4841 ; Chem. Eur. J. 2012, 18, 16136-16344) or hydrogen transfer (Chem. Eur. J. 2015, 21, 1-11). They can also be used as carbenoids precursors (ACIEE 2007, 46, 5947-50)), that can further activate borane (J. Am. Chem. Soc. 2013, 135, 8774-8777). In any of these outbreaks, the use of DFT calculation brought some crucial insight on reaction mechanisms, or fine understanding of the charge stabilization mechanism. Our project is now centered on an unexplored property of geminal dianion: their ability to bind two metallic centers through the two lone pairs at carbon in certain circumstances. Due to the close proximity of the two metallic atoms and the high electronic density at carbon, these complexes are very promising, in terms of magnetic properties as well as chemical reactivities. Furthermore, the unique possibility to synthesize heterobimetallic complexes was experimentally demonstrated quite recently in our group. This process is not mastered yet, and we expect great help from DFT modelling to orient our synthesis : influence of the nature of the chelating arms of the dianions to increase the selectivity toward a specific metal, understanding of the transmetallation mechanism to find the conditions for a trapping of transmetallation intermediates. Finally, the description of their electronic structure by DFT modeling will bring some light on their magnetic and spectroscopic properties. This new thematic in our group needs to be developed quickly, since it would be the ground of an appliance to European research council grants.

Dernières publications:

- A. Pujol, M. Lafage, F. Rekhroukh, N Saffon-Merceron, A. Amgoune, D. Bourissou, N. Nebra, M. Fustier-Boutignon, N. Mézailles; Angew. Chem. Int. Ed. 2017, 56, 12264 –12267 - **doi:** pu.doi

Étude de la réactivité et de la caractérisation des propriétés catalytiques de systèmes allant du cluster à la Nanoparticule

Projet démarré en 2014

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Iker Del Rosal**

Nanoparticles (Nps) exhibit physical and chemical properties intermediate between those properties exhibit of small molecular compounds and the bulk material, resulting from surface or quantum size effects. Special sites are also known to play a role in heterogeneous catalysis and in synthesis over nanoparticles.More efficient nanocatalysts need to be developed, yet the task of discovering novel alternatives has proven to be extremely challenging. Non-magnetic ruthenium (NPs)constitute an important class of catalysts, involved in hydrogenolysis reactions, olefin metathesis, hydrogenation of aromatic compounds, and the FischerTropsch reaction. It is a catalyst of utmost importance which deserves a deeper understanding of its surface properties under the NP state, a range of sizes with possible quantum size effects. In the same way, magnetic nanoparticles are of interest because of their outstanding magnetic properties are expected to lead to a specific catalytic behavior due to their enhanced magnetic moment, and because of their wide range of possible applications, such as data storage, spintronics etc. In this context, we plan to realise in 2014 an extended study of different magnetic and non-magnetic nanomaterials and their use in catalysis.

Dernières publications:

- Monomeric Thorium Dihydrido Complex: A Versatile Precursor to Actinide Metallacycles, G. Qin, Y. Wang, X. Shi, I. Del Rosal, L. Maron, J. Cheng, Chem. Comm., 55 : 8560 – 8563 -
- Efficient CO2 transformation under ambient condition by heterobimetallic rare earth complexes: experimental and computational evidences of a synergistic effect, L. Qu, I. Del Rosal, Q. Li, Y. Wang, D. Yuan, Y. Yao, L. Maron, Jornal of CO2 utilization, 33 : 413 – 418 -

Modélisation quantique et classique de systèmes en phase condensée par les méthodes SCC-DFTB et DFT

Projet démarré en 2013

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Jérôme Cuny**

The P1320 project entitled « Quantum and Classical Modeling of Condensed Matter Systems using the SCC-DFTB and DFT Approaches» intends to extend the expertise of the «Modelling, Aggregates and Dynamics» group of the LCPQ to the field of condensed-matter science. Three main topics are addressed within this project: - Study the influence of nuclear quantum effects (NQE) on the structural and spectroscopic properties of condensed matter systems, in particular aqueous systems. One aspect of this topic was initiated in 2013 when we combined the self-consistent-charge density-functional based tight-binding (SCC-DFTB) approach implemented in the deMon-Nano code with the i-PI code. We are now at the point where we can simulate SCC-DFTB liquid water including NQE and our aim is to extend this study to other phases of water. In parallel, we are also studying the influence of NQEs on the 17O and 1H NMR properties of liquid water at the DFT level. - Study the impact of solvent effects on the reactivity of molecular species in aqueous solution. In particular, we intend to understand the photo-reactivity of the [Ru(terpy)(bpy)(Hmte)]2+ polypyridyl complex in water using molecular dynamics simulations in combination with DFT in the excited state. More precisely, we look at determining if the reaction of [Ru(terpy)(bpy)(Hmte)]2+

with a water molecule follows a concerted or a stepwise mechanism. In the latter case, each reaction steps will be looked at. The goal of this topic is to provide a deeper understanding of the reactivity of polypyridyl complexes in water to improve their applications in medicine. - Finally, the P1320 project focuses on the proton-conduction properties of solid-state compounds to provide a deeper understanding of the transport mechanism involved in such compounds. More specifically, we intend to rationalise the influence water content and/or thermal fluctuations on proton transport in polyoxometalates and in molybdenum cluster compounds.

Dernières publications:

- J. Cuny, F. Jolibois, I. C. Gerber, Evaluation of Gas-to-Liquid 17O Chemical Shift of Water: A Test Case for Molecular and Periodic Approaches, J. Chem. Theory Comput. 2018, 14, 4041−4051 - **doi:** pu.doi
- A. de la Lande, A. Alvarez-Ibarra, K. Hasnaoui, F. Cailliez, X. Wu, T. Mineva, J. Cuny, P. Calaminici, L. López-Sosa, G. Geudtner, I. Navizet, C. G. Iriepa, D. R. Salahub, A. M. Köster Molecules 2019, 24, 1653 - **doi:** pu.doi

Propriétés moléculaires relativistes

Projet démarré en 2013

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Trond Saue**

The overall theme of the proposed project concerns the calculations of molecular properties in a relativistic framework. In the present period we will proceed along five lines of research: i) We have recently developed the calculation of expectation values at the level of 4-component relativistic coupled cluster. We will use this novel method to calibrate our DFT protocol developed for the calculation of parity-violation in chiral molecules. ii) We will carry out a benchmark study of spin-orbit splitting in the p-block atoms in response to a recent publication on this that we consider flawed. iii) We are starting a projet on the investigation of QED effects on molecular properties. We seek to develop a nonperturbative approach and expect some pilot calculations in the coming period. iv) An extension of our recently developped relativistic equation-of-motion (EOM) coupled cluster module is the introduction of core-valence separation, allowing the simulation of X-ray absorption spectra. Pilot calculations are expected. v) We are in the final stages of a project investigating the validity of the electric dipole approximation in X-ray absorption spectroscopy.

Dernières publications:

- Christopher South, Avijit Shee, Debashis Mukherjee, Angela Wilson and Trond Saue, 4-component relativistic calculations of L_{3} ionization and excitations for the isoelectronic species UO_{2}^{2+} , OUN^{+} and UN_{2} , PCCP 18 (2016) 21010 - **doi:** pu.doi
- Adel Almoukhalalati, Stefan Knecht, Hans Jørgen Aagaard Jensen, Kenneth G. Dyall and Trond Saue, Electron correlation within the relativistic no-pair approximation, J. Chem. Phys. 145 (2016) 074104 - **doi:** pu.doi

Dianions géminés et carbénoides / trimérisation vs oligomérisation de l'éthylène/ réduction de N2

Projet démarré en 2013

LHFA - Laboratoire d'Hétérochimie Fondamentale et Appliquées (UMR 5069)

Porteur de projet: **Nicolas Mézailles**

Over the past years, we have been developing the use of dianions, where the two charges are located on the same carbon atom. These highly sensitive molecules are then used to transfer electron density to metal fragments

(transition metals, lanthanides, actinides) in order to form metal carbene complexes. We are interested in probing the nature of the interaction between the M and C by experimental and theoretical methods as well as rationalizing the reactivity of the complexes. We have shown in 2017 in particular that these dianions can allow the stabilization of the first gold carbene complex. Calculations guide reactivity tests as well as further modifications of the ligand system to increase the Au=C bond strength. From another standpoint, we are interested in finding the experimental parameters that allow the selective oligomerization of ethylene catalyzed by homogeneous complexes. In order to do so, various pathways of oligomerization/polymerization have to be computed and compared. We focus on Ti and Ni complexes. Finally, we study the reduction/functionalization of N2 using designed Mo/Fe fragments. The reactivity is studied in a dual experimental / theoretical approach. Experimentally, we use a platform of the type (PP2)M, where PP2 is a tridentate phosphine ligand, to coordinate N2 in a first step. Subsequent functionalization is achieved via either electrons/electrophiles additions or additions of neutral substrates such as silanes and boranes. Our ultimate goal is to develop homogeneous catalysts for the direct incorporation of N atoms of dinitrogen into various amines.

Dernières publications:

- Angew. Chem., Int. Ed, 2018, 57, 1874 - **doi:** pu.doi
- Chem. Commun. 2018, 54, 11953 - **doi:** pu.doi

Interaction de pesticides avec les fractions minérale et organique du sol.

Projet démarré en 2012

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Fabienne Bessac**

The first molecule under study was atrazine molecule, 2-chloro-N4-ethyl-N6-isopropyl-1,3,5-triazine-4,6-diamine. It is the active substance of a pesticide which has an herbicide effect. This molecule is one member of the triazine family characterized by an s-triazine cycle. Forbidden within the European Union since 2004, it has still been used in about 80 countries all over the world and is one of the most employed pesticides. The use of atrazine is highly controversial because of its negative impact on the environment. Thus, understanding fate and transport of this compound in soils and water is of great interest. Since 2014, our work has also been dealing with metamitron (herbicide) and fenhexamid (fungicide). To start, the soil has been modeled by only the mineral part. A Ca-montmorillonite clay has been chosen. Our project uses a multiscale approach organized in four levels starting from gas phase molecular systems to condensed phase: • Isolated pesticide ; • Complexes with one or two atomic cations ; • Pesticide on dry montmorillonite ; • Pesticide on hydrated montmorillonite. In order to obtain information on the adsorption of the pesticide on a clay surface, we use the CPMD program with periodic DFT (PBE functional with a D2 dispersion correction). Static calculations and Car-Parrinello Molecular dynamics allow to access physical and chemical properties of the adsorption and desorption of pesticides in soils. Modeling such large systems of about 600 atoms (pesticide + clay surface + water solvent) demands important computing resources.

Dernières publications:

- "Pesticide interaction with environmentally important cations: A molecular dynamics and DFT study of metamitron and fenhexamid." Bastien Belzunces, Sophie Hoyau, Jérôme Cuny, Fabienne Bessac, Computational and Theoretical Chemistry 1117 (2017) 220–234. - **doi:** pu.doi
- Metamitron and fenhexamid interaction with Ca2+-Montmorillonite clay surfaces: a DFT molecular dynamics study. Bastien Belzunces, Sophie Hoyau, Fabienne Bessac, Journal of Computational Chemistry, submitted for publication. - **doi:** pu.doi

Etudes de propriétés photophysiques et photochimiques de molécules organiques

Projet démarré en 2012

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Martial Boggio-Pasqua**

In this project, we propose to study the photochemical and photophysical properties of various organic molecules with different applications in view. Two classes of organic chromophores are currently under investigation: 1) photochromic compounds (DHP/CPD, dithienylethenes, DHA/VHF, etc.) used as photoswitches 2) aromatic charged compounds of astrophysical interest Photochromism represents an increasing area of research in photochemistry because of its actual and potential applications. Photochromic molecular systems have entered the new generation of innovative functional materials with high added value. Applications are already widespread in nanosciences, biology, and photonic or optoelectronic devices as light-activated switches. However, the underlying mechanisms by which these molecular switches operate are often not fully understood. Computational photochemistry provides a very efficient tool to bring detailed insights into these mechanisms. The purpose of this part of the project is to use our expertise in computational photochemistry to rationalize original photochromic behaviors in realistic conditions and to design new systems with improved photoswitchable properties. We will investigate the photochromism of the dimethyldihydropyrene family of compounds within the framework of a starting ANR proposal called Photochromics and also naphthoquinone derivatives of dithienylethenes as part of a collaboration with the group of Dan Patel at Penn State university. Aromatic charged compounds such as polycyclic aromatic hydrocarbon (PAH) cations and fullerene cations are of particular astrophysical interests as a consequence of their detection in circumstellar environments. Notably, they have been proposed to be responsible for some diffuse interstellar bands (DIBs) and for some emission features. Our calculations aim to rationalize the photophysical properties of this type of cations and to compare with laboratory experiments carried out on these species.

Dernières publications:

- Theoretical rationalization of the dual photophysical behavior of C60+, J. Soler, R. Sarkar, M. Boggio-Pasqua, J. Phys. Chem. A 123, 2019, 1824–1829. - **doi:** pu.doi **url:** pu.open_url
- 1. Using Density Functional Theory Based Methods to Investigate the Photophysics of Polycyclic Aromatic Hydrocarbon Radical Cations: A Benchmark Study on Naphthalene, Pyrene and Perylene Cations, M. Boggio-Pasqua, M. J. Bearpark, ChemPhotoChem 3, 2019, 763–769. - **doi:** pu.doi **url:** pu.open_url

Hydrogénation catalytique de nitriles sur une surface de palladium

Projet démarré en 2012

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Iker Del Rosal**

Nitriles are important materials in the chemical and pharmaceutical industries. These materials are widely used on the manufacture, via a hydrogenation process, to their corresponding primary amines which have found widespread applications as solvents, fibers for textiles.... However, in contrast to other hydrogenation processes, which usually proceed relatively simply, in the hydrogenation of nitriles a mixture of primary, secondary and tertiary amines are formed. The generally accepted hydrogenation mechanism, proposed by J. von Braun et al. in 1923, suggests that the hydrogenation reaction involves the formation of an imine intermediate. This imine can, in addition to hydrogenation reaction which leads to the primary amine, react with the initially formed primary amines in order to, trough a reductive amination process, give the secondary and tertiary amines. However, although the formation of an imine intermediate as well as the reductive animation process involved in the hydrogenation mechanism of nitriles are generally accepted, several questions remain unanswered. The most

important controversy concerns the reactive intermediates for which no experimental evidence allows to clearly determine their nature. The present project is realized in order to shed light on this controversy, by the determination of the synthesis process of the different amines as well as the elucidation of the nature and geometry of the different surface intermediates.

Etude ab-initio des propriétés électroniques dans des systèmes de basses dimensionalités

Projet démarré en 2010

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Thierry Leininger**

The main objectives of our project are the development and the application of the Total Position Spread Tensor (TPS) (and its counterpart, the Total Momentum Tensor, TMT) to complex and extended systems. Our project is two fold. First, we will use the TPS to study some cubic systems of second row atoms, X4Y4 (X, Y= B, C, N, O and F). Secondly, we will continue our previous work to extended systems. Indeed, the ab initio study of this kind of systems by using wavefunction-type methods is giving in these last years extremely interesting results, and is opening a completely new approach for the study of solids. In this context, the problem of the periodic nature of systems that presents long-range interactions plays a central role and the TPS/TMT are certainly valuable tools to gain some physical insights on the electronic correlation. We will thus extend the applicability of these properties to periodic systems to study i) The Electric Polarizability, ii) The quantum Coulomb Interaction in an electron gas and iii) The classical Coulomb Interaction between ions in a crystalline system.

Dernières publications:

- A. Segalina, A. Francé-Monerris, M. Pastore, T. Leininger, S. Evangelisti et A. Monari, Theoret. Chem. Acc. 137, 163 (2018). Conical intersection properties unraveled by the position spread tensor. -
- A. Diaz-Marquez, S. Battaglia, G. L. Bendazzoli, S. Evangelisti, T. Leininger et J.A. Berger, J. Chem. Phys. 148(12), 124103 (2018). Signatures of Wigner localization in one-dimensional systems. -

Structure et Activité Catalytique en Chimie Organométallique

Projet démarré en 2009

LCC - Laboratoire de Chimie de Coordination (UPR 8241)

Porteur de projet: **Mary Grellier**

Our research focuses on the transition metal complex development with non- conventional coordination modes and specially the understanding of the metal-ligand interaction. One of the main research concerns the chemistry of complex M (sigma- HE) (E = H, C, Si, Ge) including one or more sigma -HE Bonds. Applications in catalysis are at the heart of our studies. The importance of DFT calculations using the Gaussian 09 software is essential for the characterization, the interpretation of the stability and reactivity of our complexes. These calculations are important to confirm our experimental observations and to model the reactivity of these compounds. Our study is divided in two parts: a) Understanding of the stability of various complexes of iron and ruthenium in association with the experimental characterization of these compounds (such as NMR predictions). b) Reactivity studies of these species from a catalytic point of view. We will calculate the energies of the different possible transitions and intermediate states in catalytic hydrofunctionnalization reactions by Iron and ruthenium complexes. We would like to develop increasingly predictive approach of calculations for selecting ligands function of the desired properties in the complexes.

Dernières publications:

- Dalton Transactions, 2018, 47, 10139-10146 - **doi:** pu.doi **url:** pu.open_url
- Organometallics, 2019, 38, 626–637 - **doi:** pu.doi

Etude de propriétés photophysiques et photochimiques de complexes métalliques photochromiques

Projet démarré en 2008

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Martial Boggio-Pasqua**

Ruthenium nitrosyl complexes have found utility in a variety of applications, such as optical switches and data storage [1], or medicine [2]. Depending on the ancillary ligands, environment, and irradiation wavelength, these complexes can undergo either intramolecular N→O linkage photoisomerization [3] or NO photorelease [4]. However, the mechanism behind these two competing processes is lacking. Preliminary results obtained by our group on the [RuClNO(py)4]2+ complex using density functional theory (DFT) points toward a complex two-photon mechanism on the lowest triplet potential energy surface [5]. A dynamical study using TD-DFT performed by the group of L. González in Vienna provides some information on the initial steps of the photorelease mechanism for a different ruthenium nitrosyl complex [6]. To unravel the photoisomerization and photorelease mechanisms and the factors governing their competition, we propose to study the photodynamics of different ruthenium nitrosyl complexes using ab initio or TD-DFT molecular dynamics (MD), including the description of the intersystem crossings (ISC) between initially populated singlet states to the lower triplet states. In 2016 and 2017, we have performed a theoretical study of the [RuClNO(py)4]2+ complex using highly-accurate ab initio multireference calculations.[7] In particular, we have described the most probable ISC pathways accounting for triplet state population. We have also computed the relevant potential energy surfaces along the N→O linkage photoisomerization pathways and interesting information has been obtained on the photoswitching mechanism of this complex, which confirms and completes our previous DFT study. TD-DFT calculations have also been performed to establish a computational protocol that will be viable for the photodynamics study.[8] In 2018, we have carried on our study of this complex by computing the NO photorelease pathways and by simulating the photodynamics of this system with "on-the-fly" nonadiabatic dynamics. The next steps concerns the inclusion of the environment effects. We need to account for the different photochemical behaviors observed in solution (NO release) and in solid phase (NO isomerization). This investigation of the environment effects will be carried out in 2019. [1] M. Imlau et al., in Nanoelectronics and Information Technology, Ed. R. Waser, Wiley-VCH, 2003, p. 659. [2] (a) E. Culotta et al., Science 1992, 258, 1862–1865. (b) J. S. Stamler et al., Science 1992, 258, 1898–1902. [3] (a) P. Coppens et al., Chem. Rev. 2002, 102, 861–883 and 1803. (b) T. A. Bitterwolf, Coord. Chem. Rev. 2006, 250, 1196–1207. [4] N. L. Fry et al., Acc. Chem. Res. 2011, 44, 289–298. [5] J. Sanz Garcia et al., Inorg. Chem. 2015, 54, 8310–8318. [6] L. Freitag et al., Phys. Chem. Chem. Phys. 2015, 17, 14383–14392. [7] F. Talotta et al., J. Chem. Theory Comput. 2017, 13, 6120–6130. [8] A. J. Atkins et al., J. Chem. Theory Comput. 2017, 13, 4123–4145.

Dernières publications:

- Adiabatic versus nonadiabatic photoisomerization in photochromic ruthenium sulfoxide complexes: a mechanistic picture from density functional theory calculations, A. J. Göttle, I. M. Dixon, F. Alary, J.-L. Heully, M. Boggio-Pasqua, J. Am. Chem. Soc. 133, 2011, 9172–9174. - **doi:** pu.doi **url:** pu.open_url
- Linkage photoisomerization mechanism in a photochromic ruthenium nitrosyl complex: new insights from a MS-CASPT2 study - **doi:** pu.doi **url:** pu.open_url

Étude théorique de la structure et réactivité d'un catalyseur greffé sur une surface de silice.

Projet démarré en 2008

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Laurent Maron**

The major disadvantage of homogeneous catalysis as well as heterogeneous is the need to remove the catalyst and the ligands (after polymerization) by tedious and expensive treatment (liquid / liquid extraction, adsorption resin, etc.). An attractive alternative is to graft the catalyst systems on insoluble solid supports such as silica or polystyrene reticulated. This technique is at the interface between homogeneous and heterogeneous catalysis, and it avoids the steps of purification of synthesized polymers and to encourage the reuse of the catalyst system. However, by supporting the catalyst on a support coordination entails a loss of control of the intermediate steps of polymerization. The study we want to do is focus on catalysis by d and/or f metal grafted complexes on silica support. So far, we have created different models of an amorphous silica surface treated at different temperatures. We showed that to the five created models, two are in agreement with experimental data obtained for a silica surface treated at 700 ° C, while five models are in agreement with the data obtained for a silica surface treated at 300 ° C. The data used for the theoretical/experimental comparisons is both structural (distance) and spectroscopic (IR and NMR). This work, conducted in collaboration with the experimental team of R. Gauvin (Université des Sciences et Technologies, Lille) and M. Taoufik (Chemistry, Catalysis, Polymers and Processes, Lyon), it is made in the context of the theory of density functional. Our studies has shown that (i) grafting plays an important role on the catalytic activity of grafted complexes compared to their homogeneous counterpart; (ii) the grafting mode it is also important and can strongly modify the catalytic activity; (iii) the NMR is a tool of choice for the characterization of possible grafting modes but also to establish a fruitful exp/théo dialogue.

Dernières publications:

- DFT study of the ring opening polymerization of epsilon--caprolactone by grafted lanthanide complexes : 2-Effect of the initiator ligand. I. del Rosal, R. Poteau, and L. Maron. Dalton Trans., 40 : 11228–11240 (2011). - **doi:** pu.doi
- Reductive CO2 homocoupling: de novo synthesis of a borylated C3 carbohydrate, A. Béthegnies, Y. Escudié, N. Nuñez-Dallos, L. Vendier, J. Hurtado, I. del Rosal, L. Maron, S. Bontemps, ChemCatChem,, accepted, 2018 - **doi:** pu.doi

Clusters et nanoparticules métalliques : structure, propriétés électroniques, spectroscopie et état de surface

Projet démarré en 2006

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Romuald Poteau**

Metal particles at the nanoscale are currently an area of intense scientific interest, due to a broad variety of potential applications and from a fundamental point of view as well. These NPs are not so easy to stabilize, owing in particular to their mutual interaction which increases their possible coalescence. A valuable strategy to synthesize colloidal NPs is the organometallic route, which involves the presence of chemical species present at the surface of the NPs. Our 2019 project consists in three main parts: (i) nanocatalyzed water splitting (Year 3) (i_a) adsorption properties of photosensitizers grafted on RuNPs (i_b) redox properties of RuNPs stabilized with terpyriridines (ii) modification of the catalytic properties of RuNPs by dilution of iron atoms (new topic started in autumn 2017, see 2017 progress report, part I, project put on hold in 2018 – so formally Year 2) (iii) ligand effect on the catalytic activity of RuNPs (new)

Dernières publications:

- R. González-Gómez, L. Cusinato, C. Bijani, Y. Coppel, P. Lecante, C. Amiens, I. del Rosal, K. Philippot, R. Poteau, Carboxylic acid-capped ruthenium nanoparticles: experimental and theoretical case study with ethanoic acid, Nanoscale 2019, 11, 9392-9409 - **doi:** pu.doi **url:** pu.open_url

- R. González Gómez, I. del Rosal, K. Philippot, R. Poteau, DFT calculations in periodic boundary conditions of gas-phase acidities and of transition-metal anionic clusters: case study with carboxylate-stabilized ruthenium clusters, Theor. Chem. Acc. 2019, 138, 95-104 - **doi:** pu.doi

Modélisation de composés de coordination et organométalliquespour la catalyse homogène et la polymérisation radicalaire contrôlée

Projet démarré en 2004

LCC - Laboratoire de Chimie de Coordination (UPR 8241)

Porteur de projet: **Eric Deydier**

Our computational work is directly connected with the experimental studies going on in our research group, which are centered on homogeneous catalysis and on controlled radical polymerization. It involves the optimization of molecular geometries (global and local minima, transition states when dealing with the study of reaction pathways or catalytic mechanisms, "minimum energy crossing points" when dealing with reaction with a change of spin states), with computation of the energy and of the normal modes of vibration for compounds containing in most cases only one heavy atom (transition metal) plus a certain number of lighter atoms. The calculations may need hybrid QM/MM methods, but in certain cases a full QM treatment is necessary. The group research activity is organized along two distinct topics: (i) controlled radical polymerization; (ii) homogeneous catalysis.

Dernières publications:

- Macromolecules 2019, 52, 3252–3256 - **doi:** pu.doi
- Org. Chem. Front. 2019, 6, 852-857 -

4.6 Mécanique des structures

Lightning strike on composite fuselage

Projet démarré en 2019

ICA - Institut Clément Ader

Porteur de projet: **Christine ESPINOSA**

The lightning damage mechanism for carbon laminate structures like aircraft fuselage is a complex multiphysical phenomenon. The lightning current entering into the surface metallic protection, called LSP (Lightning Strike rotection) and the carbon plies generates Joule's effects and magnetic forces which both induce mechanical forces and surface explosion that has a significant mechanical impact. After a large explorative experimental campaign, and some computation related to explosion and plasma effects in mettallic meshes, it is now necessary to compute the damage generated by a high current injection on a CFRP structure. This will use estiùations of explosive load induced by the metallic protection vaporization during a typical lightning strike current injection.

Multimaterial balistic shield structure

Projet démarré en 2019

ICA - Institut Clément Ader

Porteur de projet: **Christine ESPINOSA**

For the purposes of light weighting body armours, studies are being conducted on multi-materials protective systems composed of alumina at the front face and ultra-high molecular weight polyethylene (UHMWPE) laminated composite at the rear face. During an impact on the proposed structure, the ceramic front panel erodes and fragments the projectile, while the composite supports the ceramic and absorbs the residual kinetic energy after the fragmentation of the ceramic and the projectile. After the impact, damages are visible on both the ceramic and the laminated composite. This work aims at identifying and characterize the different damage mechanisms around the point of impact which will help to assess ballistic performance of the ceramic/composite armour against piercing projectile (AP). However, a ballistic protection is composed of several juxtaposed tiles, to limit the crack spread to a smaller volume of ceramic. The tiles are thus confined, which modifies the fracture and deceleration mechanisms of the projectile. Impact tests in different configurations are required and presented in this paper. The distributions of the morphology and of the size of fragments are analysed.

Simulations de l'instrument SVOM/ECLAIRs et caratérisation de la caméra X/gamma

Projet démarré en 2019

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **laurent bouchet**

The Space Variable Object Monitor (SVOM) to be launched in end of 2021 is a Chinese-French space mission for the study of Gamma-Ray Bursts (GRB). The coded-mask imager ECLAIRs is the leading instrument for the detection and first localization of GRBs onboard SVOM. This camera is developed by a consortium of several French labs under the science lead of IRAP and the supervision of CNES. We are currently manufacturing the various sub-systems for the camera flight model. The calibrated instrument is expected to be delivered in China at the beginning of 2021 to be integrated on the spacecraft. Beforehand, a series of performance and calibration measures of the subsystems and the whole camera will have to be carried out in our testing bench using radioactive sources (starting from the end of 2019). Our project schedule is very tight to successfully carry out the various instrumental activities up to the instrument delivery in 2021. So, we need to craft the calibration campaigns in detail by fine-tuning every calibration test. To do so, we developed a detailed Monte-Carlo simulation software, based on GEANT4 (a CERN toolkit to simulate the radiation-matter interactions) to compute the various photon and particle interactions with the camera's body. We successfully ran this software on an IRAP server to analyze data collected on a prototype of the detection plane in 2019. However, the performed simulations were rather basic and do not meet the level of accuracy needed for the calibration of the flight-model. To improve this, we need to consider a larger number of incoming photons. This will in turn result in a prohibitive computing time on our server; which will prevent us fully exploring all the expected testing configurations. However, we can take advantage of the latest developments of the GEANT4 software, which now enable scalable parallel implementations. Therefore, we request 300000 hours on the CALMIP servers to run a set of simulation that will serve to properly calibrate the ECLAIRs detection plane and the whole camera.

Identification de paramètres pour le modèle thermodynamique du système Cu-Fe-H2SO4-H2O

Projet démarré en 2018

LGC - Laboratoire de Génie Chimique (UMR 5503)

Porteur de projet: **Laurent Cassayre**

Our research project focuses on the process of dissolving a copper ore in sulfuric acid, which is part of the process of producing metallic copper from ore, in order to find the optimal conditions (improve the extraction yields and minimize the acid consumption). The approach consists in establishing a thermodynamic model for the description of the complex system Cu-Fe-H2SO4-H2O. The free PhreeqC geochemical computation software allows the

calculation of thermodynamic equilibria involving electrolytic aqueous phases. We have selected the SIT model (Specific ion Interaction Theory), which describes the activity coefficients of aqueous ions notably by taking into account the short range interactions between ion pairs i and k thanks to a parameter εi,k (T). The work in progress consists of identifying the values of the parameters εi,k over the temperature range 25-90 ° C. We estimated at approximately 10 the number of interactions to be considered in describing the full system. The principle adopted for the determination of the parameters is, for each temperature step, to vary the values of each εi,k in a fixed range, to calculate the thermodynamic equilibrium, and to minimize the difference between all calculated values and an experimental data set. The determination of the interaction parameters has been initiated on the H2SO4-H2O subsystem, with two interaction parameters. To do this, we have developed a procedure based on the use of a Fortran code that calls the Phreeqc software. This approach made it possible to determine the two interaction parameters as a function of temperature, with calculation times of a few hours. Further work on the Fe-H2SO4-H2O subsystem, however, comes up against the length of the calculations. Thus, in the current configuration (4 pair interactions), a calculation takes about ten days, which is very penalizing to test our approach. The present request to Calmip therefore aims to allow us to progress in our modeling work, by reducing the computation time. We estimated it at 50,000 hours, which corresponds to about 200 computational configurations.

Optimisation topologique de la structure d'attache moteur voilure

Projet démarré en 2018

ICA - Institut Clément Ader

Porteur de projet: **Christian Gogu**

Engine deformations during operation of an aircraft have a sensible impact on the engine's fuel consumption and are thus are an increasing concern for both engine and aircraft manufacturers. The tip-clearance, defined as the radial gap between the blade tip and the engine casing, can show small variations induced by aircraft maneuvers both on the ground and in flight. These variations can produce increased tip leakage flow, secondary flows and vortex losses that can sensibly increase the engine trust specific fuel consumption (TSFC). The topology of the structure connecting the engine to the rest of the aircraft through the wing pylon will directly impact the tip clearances and thus the thrust specific fuel consumption. The project aims at carrying out high fidelity topology optimization of the engine-pylon structure in order to minimize the TSFC. A specific topology optimization framework was developed by the team for this purpose, involving static condensation of the aircraft engine model, mesh coupling of the design zone and condensed engine model, adjoint sensitivities for solving the optimization problem. A main challenge in obtaining high fidelity designs resides in increasing the number of the degrees of freedom (DOF) considered in the design zone (tens or even hundreds of millions of DOFs). To achieve this, the project builds upon recent developments in highly parallel topology optimization frameworks that were recently able to achieve up to a billion DOFs in a HPC environment on simpler minimum compliance topology optimization problems. Upon completion the project is expected to provide innovative high fidelity structural designs for the engine wing assembly that will help reduce the lifetime fuel consumption of future aircraft.

Traitement numérique de la localisation et de la rupture dans les matériaux structuraux sous sollicitations sévères

Projet démarré en 2016

ICA - Institut Clément Ader

Porteur de projet: **Patrice Longère**

Under severe loading, including shock and impact, structural materials are subjected to large strain, high strain rate and temperature rise, at least locally. The resulting thermal- and/or damage induced-softening may lead to

strain localisation in narrow bands and further fracture. The standard finite element method is known to suffer from pathological mesh dependence in the softening regime. There exist different technique aiming at attenuating this mesh dependence. The one adopted herein consists in embedding the band of localised deformation in the representative volume element and developing enriched constitutive models and/or finite element kinematics in user subroutines for solving complex initial-bounadry value problems. Those developments are currently in progress in the framework of Johannes Wolf and Dorothy Hannah-Lois PhD studies.

Dernières publications:

- H.L. Dorothy and P. Longère. Modelling of high strain rate Adiabatic Shear Banding induced failure: a comparison of two approaches. International Journal of Impact Engineering. 110, 219-227. 2017 - **doi:** pu.doi

Amélioration des méthodes de prédiction du glissement dans les assemblages vissés dû à des chargements thermoélastiques et vibratoires

Projet démarré en 2015

ICA - Institut Clément Ader

Porteur de projet: **Alain Daidié**

The thesis entitled "Improving prediction methods of the slip in screw connections due to thermo- elastic and vibratory loads" is a continuation of a work initiated at Icam Toulouse. It is followed by CNES and Thales Alenia Space and started in September 2014 at the Icam Toulouse Mechanics Department. The main objective of the thesis is a better prediction of the slip in screw connections (conventional screws , screw / nut) for several types of space applications. First, we aim to reduce the size of connections to gain mass to improve mission costs and / or increase the payload. On the other hand , the actual stiffness of the screw connections have to be determined according to their application , in order to improve the finite element model representing the behavior of the complete structure . Slip can have several more or less important consequences. For example , in the case of an observation telescope, the performance of the equipment may be affected by a single micro-slip . In the case of a structural screw, sliding can induce a change in the modal behavior of the equipment involved and lead to critical eigenmodes couplings between the equipment and the satellite. Ultimately, this thesis aims to provide comprehensive and optimized methods for calculating slip . In practice, this involves the construction of detailed finite element models to correctly model the mechanisms of sliding, the realization of a substantial number of tests to compare modelizations to practice and programming of advanced slip prediction tools.

Dernières publications:

- R. Thanwerdas, E. Rodriguez and A. Daidié. Stiffness and slip laws for threaded fasteners subjected to a transversal load. Proceedings of International Joint Conference on Mechanical Design Engineering & Advanced Manufacturing (JCM2016) p.517-526, 2016 - **doi:** pu.doi
- R. Thanwerdas, E. Rodriguez, A. Daidié, M. Heim and C. Fabries. Industrial Equivalent Modelling of a Screw Assembly Subjected to a Thermal Load. Proceedings of 14e European Conference on Spacecraft Structures, Materials and Environmental Testing (ECSSMET) p.1-15, 2016 -

Étude des pièces composites de formes complexes /// Étude des assemblages collés

Projet démarré en 2012

ICA - Institut Clément Ader

Porteur de projet: **Steven Marguet**

This thesis work deals with the characterization and the modeling of the mechanical behaviour up to failure of laminated composite structures involving complex shapes. One of the major failure modes of laminated composite parts is the demalination. A way to prevent this issue is to design the parts in such a way that avoids the occurence of these phenomenon. Double curved parts present these suited characteristics in terms of prevention of delamination. The study is going to follow three steps: - parametric experimental study on elementary coupons to identify and understand the phenomena - characterization and modeling of the local orientation of the fibers of the composite - modeling of the whole part with suited mechanical behaviours

Dernières publications:

- B. Valès, S. Marguet, R. Créac'hcadec, L. Sohier, J.-F. Ferrero, P. Navarro. An experimental method dedicated to the dynamic characterization of structural adhesives under drop weight conditions, International Journal of Adhesion and Adhesives, Volume 90, 2019, Pages 106-125. - **doi:** pu.doi
- S. Arki, J.-F. Ferrero, S. Marguet, J.-M. Redonnet, A. Aury, Strengthening of a curved composite beam by introducing a flat portion, Composite Structures, Volume 222, 2019. - **doi:** pu.doi

MOdélisation CInétique de Plasmas sur Supercalculateur dans le contexte de sources d'ions - MOCIPS

Projet démarré en 2011

LAPLACE - Laboratoire Plasma et Conversion d'Energie (UMR 5213)

Porteur de projet: **Laurent Garrigues**

Most of the time low temperature plasmas (LTP) can be simulated using fluid approaches because the distance between two collisions is orders of magnitude lower than the characteristic length of the system. At low pressure, when the number of collisions becomes rare, fluid approaches fails. One way to simulate LTPs at low pressure is to solve the Boltzmann equation using kinetic-particle approaches, where the unknown is the distribution function of the particles that constitute the plasma in phase space. In particle methods used in LTPs, the computational domain is divided in cells. The plasma (electrons and ions) is simulated with a larger number of particles. From a given distribution of electromagnetic fields, particle trajectories are integrated. The charged densities are calculated on grid nodes from the positions of all the particles. From charged particle distributions, the electromagnetic fields are obtained solving Maxwell equations. Collisions between charged particles and background gas are treated with statistical methods. This technique is referred as Particle-In-Cell Monte Carlo Collisions (PIC-MCC) in the literature. PIC-MCC methods are well suitable for parallel computing. PIC-MCC methods are developed and used in the LAPLACE laboratory in the GREPHE research group in the context of projects with CNES and French Start-ups for plasma propulsion for satellites, EUROfusion for ion sources of the DEMO neutral beam injector. PIC-MCC methods are used to better understand the electron transport across magnetic field barriers in these ion sources. This technique has been already successfully used on the EOS cluster through the study of electron transport in a Hall Thruster for plasma propulsion, extraction of negative ions in the ITER context (a new type of source will be now studied). A new topic concerns the applicability of sparse grid techniques to PIC-MCC method to reduce computational time in the context of low temperature plasmas. The goal of this project is to use a parallel hybrid OpenMP/MPI PIC-MCC model in a 2D, 2.5D and 3D versions.

Dernières publications:

- J. P. Boeuf and L. Garrigues, "ExB Electron Drift Instability in Hall Thrusters: Particle-In-Cell Simulations and Theory", Physics of Plasmas 25, 061204 (2018) - **doi:** pu.doi
- T. Charoy, J. P. Boeuf, A. Bourdon, J. A. Carlsson, P. Chabert, B. Cuenot, D. Eremin, L. Garrigues, K. Hara, I. D. Kaganovich, A. T. Powis, A. Smolyakov, D. Sydorenko, A. Tavant, O. Vermorel, and W. Villafana, "2D Axial-Azimuthal Particle-In-Cell Benchmark for Low-Temperature Partially Magnetized Plasmas", Plasma Sources Sci. and Technol. 28, 105010 (2019). - **doi:** pu.doi

Modélisation au crash de structures composites élémentaires

Projet démarré en 2010

ICA - Institut Clément Ader

Porteur de projet: **Samuel Rivallant**

Thanks to their high strength-to-weight ratio, composite materials are widely used in the field of transport and especially in aerospace applications, where weight savings are important. But specificity and complexity of composite fractures modes make difficult the prediction of the mechanical behaviour of composite structures subjected to crush loading. Numerous studies have been done in the last decades and the interest in crashworthiness is still present as show the recent works on the subject. But there is still a lake in numerical simulation. Most of the models developed in the last few years are based on global tests characterisation that make the model depend on global parameters, which do not permit to have predictive models. Some models are based on material characteristics, but often need an a priori knowledge of the crush damage mode developed in the crush front. The challenge today in crashworthiness simulation is then to be able, from elementary material characterisation data, to predict both crush damage modes and energy absorption in any structures. This study propose a finite element model for simulation of crushing of composite plates and sandwich structures under impact.

Dernières publications:

- ISRAR H.A.. : Etude expérimentale et numérique de l'écrasement de stratifiés composites à base de fibres de carbone. Thèse de doctorat de l'Université de Toulouse, soutenue le 21/02/2014. -
- - Wilhelm A. Rivallant S. Ferrero JF. : Study of the deformation of a sandwich shield subjected to bird impact: A behaviour analysis tool using vector decomposition, Journal of Sandwich Structures and Materials, 2018 online -

Modélisation d'endommagement sur plaque stratifiée composite

Projet démarré en 2010

ICA - Institut Clément Ader

Porteur de projet: **Christophe Bouvet**

The project presented here is focused on the numerical modeling of composite laminates made of unidirectional plies. The objective is to develop predictive models of impact and post-impact residual strength. At the same time, experimental studies are conducted to investigate the damage scenario during impact and compression after impact (CAI), and provide experimental data to validate the simulations. A finite element modeling with a Discrete Ply Model (DPM) approach is performed based on previous work done at the laboratory. This approach allowed us to simulate damage development in composite structures for aeronautical applications. This approach was applied during the phds of Benjamin Ostré and Hakim Abdulhamid for impact solicitations and is currently used during the phds of Nicolas Dubary, Pablo Garcia Perez and Fadhel Chatti.

Dernières publications:

- Dubary N., Bouvet C., Rivallant S., Ratsifandrihana (2018) Damage tolerance of an impacted composite laminate, Composite Structures, Vol. 206, pp. 261-271 - **doi:** pu.doi
- Chatti F. ., Bouvet C., Poquillon D, Michon G. (2018) Numerical modelling of shear hysteresis of entangled cross-linked carbon fibres intended for core material, Computational Materials Science, Vol. 155, pp. 350-363 - **doi:** pu.doi

Flux réactif activé par décharges couronne

Projet démarré en 2010

LAPLACE - Laboratoire Plasma et Conversion d'Energie (UMR 5213)

Porteur de projet: **Olivier Eichwald**

Le projet concerne l'optimisation des réacteurs plasmas utilisant des décharges électriques de type couronne pour la décontamination biologique et/ou chimique de l'air ou de l'eau. Ces réacteurs sont très efficaces lorsque la concentration des polluants est très faible (quelques centaines de ppm) dans le mélange gazeux. Quelques soient leurs configurations, on distingue deux phases dans les procédés corona qui se suivent et se répètent en permanence. Ces deux phases sont caractérisées par des échelles de temps et d'espace très différentes : - Dans la première phase, dite phase de décharge et qui dure quelques centaines de nanosecondes, des ramifications de décharges filamentaires (de diamètres de quelques dizaines de microns) génèrent par collisions entre électrons énergétiques et molécules du gaz des radicaux chimiquement actifs dans des proportions similaires à celles des polluants. - Dans la seconde phase, dites phase de post-décharge et qui dure quelques millisecondes, les radicaux sont transportés par le gaz réactif en écoulement, diffusent et réagissent avec les polluants pour les transformer en espèces inoffensives. L'optimisation des procédés plasmas de type corona passe par l'estimation de la production et de la répartition des radicaux formés durant les phases de décharge et par une meilleure compréhension des mécanismes physico-chimiques de transformation des polluants lors des phases de post-décharge. L'étude par la simulation de la première phase fait l'objet de demandes régulières dans le cadre du projet CALMIP (Projet « Plasma Removal »). Ce nouveau projet concerne l'utilisation du logiciel FLUENT pour la simulation instationnaire d'un écoulement gazeux réactif activé régulièrement par des décharges filamentaires de type couronne.

Dernières publications:

- M. Meziane, O. Eichwald , J.P. Sarrette , O. Ducasse and M. Yousfi, "Multi dimensional simulation of a polluted gas flow stressed by a DC positive multi-pins corona discharge reactor", International Symposium on Non-Thermal Plasma Pollution Control Technology & Sustainable energy, ISNTP 8, 25-28 june 2012, Camaret, France (Invited Conference) -
- J.P. Sarrette, O. Eichwald, O. Ducasse, "Electro-hydrodynamics simulation of ozone production in a multi pins to plane corona discharge reactor", 22nd International Conference on Gas Discharges and Their Applications (GD 2018), Novi Sad Serbia, September 2-7, 2018 -

Impact sur structure composite (pales d'hélicoptère)

Projet démarré en 2009

ICA - Institut Clément Ader
Porteur de projet: **Pablo Navarro**
This project aims to study the degradation of helicopter blades in composite material subjected to high velocity impact loadings. The final objective is to develop a strategy for modeling the physical phenomena involved in order to be able to predict the residual state of a blade after impact. The numerical model must be validated by performing impact tests. The phenomena are strongly non-linear, and many variable are required to characterize the state of the components of the composite blade. A significant computing power is indispensable to progress at this stage.

Dernières publications:

- A. Rogani, Pablo Navarro, Steven Marguet, Jean-François Ferrero, C. Lanouette. Tensile post-impact behaviour of thin carbon/epoxy and glass/epoxy hybrid woven laminates – Part II: Numerical study. Composite Structures, Elsevier, 230, p.111455 -

- A. Rogani, Pablo Navarro, Steven Marguet, Jean-François Ferrero, C. Lanouette. Tensile post-impact behaviour of thin carbon/epoxy and glass/epoxy hybrid woven laminates – Part I: Experimental study. Composite Structures, Elsevier, 230, p.111508 -

Plasma ReMoval

Projet démarré en 2006

LAPLACE - Laboratoire Plasma et Conversion d'Energie (UMR 5213)

Porteur de projet: **Olivier Eichwald**

The 3D-Streamer project aim is to optimize plasma reactors (corona discharges) in the framework of biological and/or chemical decontamination of air or water (acting in surface). To optimise the plasma reactor, we have to estimate the production of radical species (O, OH, N, HO2) within the discharges channels produced during the discharge period by electronic impacts on the gas molecules (N2, O2, CO2, H2O). The radical production is important to quantify, since radicals participate to the transformation of oxides and bacteria, during the post-discharge. But, experimentally it is very difficult to obtain the radical concentration and their nature within the channels, due to their thickness (about 10µm), formation velocity (about 10ns on 1cm), and due to its unpredictable localisation. Thus, the objective is to estimate the radical production within the plasma channels, during the discharge period by means of modelling. Then, indirectly, the numerical results (species concentration, but also nature and chemical scheme) are experimentally validated with an electric diagnostic and an optical one.

Dernières publications:

- O. Ducasse, J-M. Plewa, O. Eichwald, P. Dessante, C. Jacobs, N. Renon and M. Yousfi, "Simulation of 3D Streamer branching using High Performance Computing", Conference SFE, Grenoble -
- O. Ducasse, J-M. Plewa, O. Eichwald, "3D Streamer Simulation in a point to plane configuration", Conference GD2018, Novi Sad -

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4.7 Physico-chimie des matériaux

Atomic structure of Size-selected Ag clusters

Projet démarré en 2019

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Nathalie Tarrat**

The atomic structure and stability of silver nanoparticles influence their toxicity. For example, a shape dependence of the toxicity of Ag nanoparticles to human alveolar epithelial cells has been shown [Particle and Fibre Toxicology, 8:36, 2011]. Another area of research for which atomic structure is expected to be important is catalysis. Ag nanoparticles are catalysts for ethylene expoxidation and it has been shown that their catalytic activity is dependent on both size and shape [ChemCatChem, 2(1):78–83, 2010]. In regard to shape dependence, the packing of surface facets is considered to be a key factor, highlighting the importance of an understanding of atomic structure. By combining experiments and theoretical approaches, we aim at addressing the issue of determining the ground state structure for specific cluster sizes (concentrating on the catalytically active size regime) and to rationalize it. This will be achieved experimentally through the production of highly size-controlled cluster samples, and the use of electron-beam manipulation and in-situ heating in an aberration corrected STEM (R. Palmer team, Swansea Univ.) and theoretically through an extensive study of regular structures of clusters in a size range up to 1400 atoms. The theoretical studies reported so far in the literature have not been able to determine the transition zones, in terms of size, between the different equilibrium structures. Our hypothesis is

that the determination of the simple cohesion energy used so far to compare the stability of clusters is insufficient, and that it is also necessary to take surface energies of the nanoparticle into account. A systematic study of different cluster sizes will allow us to test our hypothesis. These calculations will be carried out at CALMIP (N. Tarrat) and in the ENS Lyon calculation mesocenter (D. Loffreda).

Simulations micromagnétiques de réseaux ultradenses de nanofils magnétiques

Projet démarré en 2019

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Thomas Blon**

Après plusieurs années de projet Calmip nous n'avons pas renouvelé le projet lors de la dernière session car le doctorant arrivait au terme de son doctorat. Néanmoins, entre temps nous avons décidé qu'il nous fallait ajouter des résultats de calculs pour affiner les résultats obtenus. Ainsi nous sollicitons un projet test afin de poursuivre le projet 16037 qui concerne des simulations micromagnétiques de réseaux de nanofils de cobalt en interaction.

Dépôt de Cr sur substrats de zyrconium : détermination de données énergétiques associées par DFT

Projet démarré en 2019

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)

Porteur de projet: **Thomas Duguet**

This application is part of a collaborative project to study the deposition of amorphous chromium carbides in 4 m long and 8 mm in diameter zyrcalloy tubes (nuclear fuel bundles) by DLI-MOCVD (Direct Liquid Injection MetalOrganic Chemical Vapor Deposition). The chromium film should be uniform but the length and the high aspect ratio of the tubes represent an important processing challenge. Thus, CFD calculations (Computational Fluid Dynamics, made at SiMAP in Grenoble) are performed to guide experiments in this objective of uniformity. Hence, they need accurate energetic parameters to describe the deposition mechanisms. We want to calculate, using the density functional theory, new energetic data related to the reactions implemented in the CFD simulations. This in order to improve the current CFD simulations. This is the objective of the present application for computational time. Experimentally, the precursor is the bis (ethylbenzene) chromium (BEBC) molecule. Under the right conditions of flow, pressure and temperature, it is completely vaporized, and transported downstream to the reactor. When the precursor reaches the inside of the furnace, it is decomposed to form amorphous Cr carbide, α-CrCx on the susbtrate. The current CFD model includes decomposition of all BEBC in the gas phase prior to reactive adsorption of the decomposition products on the zirconium (Zr) or zyrcone (ZrO2) surface. It seems useful to add, in the CFD model, energetic terms related to the adsorption and/or heterogeneous decomposition of BEBC. This is the purpose of the DFT calculations for which we apply for hours.

Micromagnetic and atomic spin simulations of magnetic skyrmions for information technology applications

Projet démarré en 2019

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Anne Bernand-Mantel**

Magnetic skyrmions are topological solitons made of a swirling spin textures in ferromagnetic materials. The recent observation of stable skyrmions at room temperature and the demonstration of their current induced displacement with low current densities has attracted a strong interest in the spintronics community and applications for information technologies are considered (memory, logic, neuromorphic or stochastic

computing,…). We are currently funded by the US government via a DARPA project and several ANR projects to work on this topic. The aim of the present work is to explore an emerging direction for skyrmions which is potentially promising for applications. Previous theoretical works on skyrmions has focused on systems where the long range dipolar effects where neglected. This is partly related to the fact that such long range effects are challenging to calculate in a mathematical point of view. Consequently, the role of long range interactions has been overlooked as well as their potential for the stabilization of nanometer scale skyrmions. We have recently work on analytical modeling to address the problem in 2D. Recent theoretical and experimental results shows that 3D modeling is necessary to address the most relevant case for applications. In the present project, we want to address this challenging micromagnetic 3D problem involving long range interactions using existing numerical simulations programs. We have selected two open source programs which are particularly relevant both in the physics point of view and also due to their relevance as regards the use of the supercalculator Olympe (parallel and GPU computing). This programs are : Mumax3 which is a GPU-accelerated micromagnetic simulation program and FIDIMAG an atomic spin simulation program with the with the nudged elastic band method implemented.

Propriétés électroniques et magnétiques aux interfaces métal/oxyde

Projet démarré en 2019

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Rémi Arras**

This project consists in using first principles methods to calculate the electronic structure in the vicinity of metal/oxide interfaces. The performed calculations will enable to calculate relevant properties such as the Schottky barrier height resulting from the band alignement at the interface or the magnetoelectric coupling in the case of interfaces between a ferromagnetic metal and a ferroelectric insulating oxide. The presence of structural defects (in particualar oxygen vacancies or the oxidation of the metallic layer) will be taken into account to get the most precise description of such interfaces.

Dernières publications:

- R. Arras and S. Cherifi-Hertel, ACS Appl. Mater. Interfaces 11, 34399 (2019) - **doi:** pu.doi

Approche multi-méthodes pour l'exploration du paysage énergétique dans les systèmes complexes

Projet démarré en 2018

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Marie Brut**

This project supports a new PhD thesis that started in September 2018 (Lionel Foulon). It aims at coupling to the algorithm "FleXible" (based on the Static Modes (SM) approach developed at LAAS-CNRS) with DFT calculations, in order to guide them and save human and computing time and resources during the exploration of energetic landscapes in complex systems. The SM method has been developed and used until now to study macro-biomolecules and the complexity associated to their energy landscapes. We wish now to test its capabilities to explore the energy landscape and optimize the choice of significant atomic events. Such developments will be applied to various biohybrid and inorganic systems, and are expected to participate in a new predictive, innovative and multi-scale approach, adapted to complex systems while keeping a reduced calculation time.

Manipulation de la Charge de nanoparticules métalliques sur des surfaces isolantes

Projet démarré en 2018

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **David MARTROU**

Electron or hole transfer processes in semiconductor or insulating interfaces, which are sandwiched between metallic electrodes, are important elementary processes in any kind of micro- or nano-electronic component. To reach a level of information at the atomic level it is necessary to work on model systems composed of metallic 3D nanoparticles or 2D islands (indistinctly labelled NP in the following) which are supported on an insulating layer, and with non-contact AFM (nc-AFM) and related techniques like EFM and Kelvin probe force microscopy (KPFM) which allow explicitly charging metal NPs and quantifying their charge via measuring the electrostatic interaction between the tip and the surface. The objective of this project is to study CT processes (1) between a metallic NP and a conducting support through an insulating thin film of thickness t (1 nm< t <100 nm) and (2) between two NPs under the influence of the insulating film. Such CT processes will be studied in dependence on the film thickness and structure (monocrystalline, polycrystalline, amorphous), and on the NP morphology (e.g., size). In an ideal, defect-free film, CT mechanisms involve tunnelling or internal field emission. They depend on the electronic structure of the insulating film but also on the metal-insulator interfaces where, even in the absence of extrinsic defects, specific states (e. g., metal induced gap states (MIGS) or insulator surface states) can play a role. Modelisation and theoretical calculations will be used to assist experiments describing and predicting charge/discharge phenomena of NPs. In particular the calculations will consider two systems: 2D Au islands on AlN(0001) and Au or Pd NPs on MgO(001) for which preliminary experiments suggest that charge can be injected from the AFM tip in a controlled way. The understanding gained in the study of these systems will be used to interpret same experiments for metal NPs grown on amorphous hafnium oxide (hafnia, HfO2) films.

Dernières publications:

- Giant (12×12) and (4×8) reconstructions of the 6H-SiC(0001) surface obtained by progressive enrichment in Si atoms David Martrou, Thomas Leoni, Florian Chaumeton, Fabien Castanié, Sébastien Gauthier, and Xavier Bouju Phys. Rev. B 97, 081302(R) (2018) - **doi:** pu.doi
- Stabilization of Au Monatomic-High Islands on the (2×2)−Nad Reconstructed Surface of Wurtzite AlN(0001) Benoit Eydoux, Bulent Baris, Hassan Khoussa, Olivier Guillermet, Sébastien Gauthier, Xavier Bouju, and David Martrou Phys. Rev. Applied 8, 044002 (2017) - **doi:** pu.doi

Étude des couches minces nanocomposites à base de nanoparticules d'Ag enrobées dans la silice pour des propriétés antimicrobiennes contrôlées

Projet démarré en 2017

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Magali BENOIT**

This project aims to study nanocomposite thin films based on Ag nanoparticles coated in silica for controlled antimicrobial properties. Metallic nanoparticles, in particular Ag nanoparticles (AgNPs), are known for their chemical activity but also for their plasmonic properties. In order to control their interaction with the environment and to protect them from rapid oxidation, one strategy is to coat them. Coatings containing an antibacterial agent such as AgNPs have the potential to simultaneously exhibit a high antibacterial efficiency and a high exaltation of the vibrationnal and luminescent signals originating from molecules located in their vicinity. It is precisely this potential that we wish to exploit in this project by means of specific dielectric layers containing AgNPs. In this context, small AgNPS (<20 nm) coated in silica matrices were manufactured at CEMES. By studying their eco-toxicity (by measuring the inhibition of photosynthesis of green algae), it has been shown that the release of silver atoms is controlled by the depth at which the AgNPs are embedded in the silica host matrix. However, mechanisms for the release of Ag ions and their diffusion through the thin layer of silica are not well understood. The objective of this project is therefore to provide some answers to these questions by performing simulations at the atomic

scale. In particular, we intend to model the SiO2/Ag interface for more or less hydrated silicas in order to study the influence of the water content on the diffusion mechanisms of the Ag ions. The SiO2/Ag interfaces are prepared using classical molecular dynamics simulations, then they are annealed by ab initio molecular dynamics in order to obtain more reliable structural characteristics of the interface as well as its electronic properties. The calculation of the spectral signatures of the different chemical species present at the interface can also be envisaged for the purpose of a direct comparison with experimental results. Finally, once the interfaces are characterized, we intend to study the diffusion mechanisms of the different chemical species involved in the release of Ag ions through the silica matrix.

Dernières publications:

- H. Balout, N. Tarrat, J. Puibasset, S. Ispas, C. Bonafos, M. Benoit, ACS Appl. Nano Mater. 2019, 2, 8, 5179-5189 - **doi:** pu.doi **url:** pu.open_url

Modélisation des processus physico-chimiques liés au water-splitting pour la production d'hydrogène

Projet démarré en 2017

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Alain Esteve**

The photo-induced splitting of water molecules using sunlight to produce hydrogen is currently attracting interest as a long term technological route, with the potential for low to zero greenhouse gas emission. Our goal is to support this technological development, and particularly LAAS-experiments on this subject, by addressing fundamental issues at the core of the design of optimized devices. During the year 2017, we will first focus on the basic understanding of the chemistry of water dissociation on neutral ZnO model-surfaces (polar Zn or oxygen terminated surfaces, orientation, hydroxylated surfaces, surface defects) to draw scenario for H2 or/and O2 production. Because of the current progress in our team to provide a triptych system composed of a semiconductive surface, plasmonic nanoparticles and a photosensitizer, we will provide calculations sheding light into the various interfaces that will be generated by this hierarchical nanostructure.

Dernières publications:

- Water dissociation and partial hydroxylation of perfect and defective polar ZnO model-surfaces, Mathilde Iachella, Jeremy Cure, Mehdi Djafari Rouhani, Yves Chabal, Carole Rossi, Alain Estève ACS J. Phys. Chem. C 122 (38), 21861 -

Structure atomique et conductivité électrique de matériaux pour mémoires à changement de phase

Projet démarré en 2017

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Alain Claverie**

Ce projet va probablement faire intervenir un stagiaire de 5ème année INSA ou un stagiaire M2 de l'UPS (un sujet de stage vient d'être proposé aux étudiants sur ce thème). L'étudiant recruté commencera son stage en 2017. Nous allons nous concentrer sur l'étude du lien entre la structure atomique et chimique locale de composés à changement de phase dont la composition est proche de celle de Ge2Sb2Te5, et les propriétés électriques de ces composés, en particulier leur conductivité électrique. Il s'agira de comprendre si la conductivité peut être ajustée via le désordre d'alliage (lorsque les conditions de synthèse ou les traitements termiques sont telles qu'une proportion non négligeable d'atomes sont sur des anti-sites), via la composition chimique globale (écarts à la stoïchiométrie de Ge2Sb2Te5) ou lorsque la successions des plans cristallins compacts (ainsi que leur composition chimique) est intermédiaire entre celle correspondant à la phase cubique et celle correspondant à la phase

hexagonale. La structure cristalline des ces phases cristallines et de leur écart à l'ordre parfait sera étudiée soit dans des supercellules (avec les codes Wien2k et Vasp, ce qui donnera accès aux longueurs de liaison chimique précises qui peuvent changer d'un site atomique à l'autre, en fonction de la nature précise des premiers voisins qui peut être modifiée par le désordre) soit par la méthode CPA qui permet d'étudier le cas de systèmes dans lequel le désordre atomique est parfait. La conductivité électrique sera calculée à l'aide du code SPR-KKR.

Simulations de l'adsorption des ions dans des carbones poreux modèles pour étudier les relations structure – performance dans les supercondensateurs

Projet démarré en 2017

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)

Porteur de projet: **Céline Merlet**

Supercapacitors are of great interest as energy storage systems because they exhibit very high rates of charge/discharge, long cycle lifes, and they are made of cheap and light materials. These attractive properties arise from the electrostatic nature of the charge storage which results from ion adsorption in the electrode pores. Recently, it was demonstrated that ions can enter pores of sub-nanometer sizes leading to a huge increase of capacitance. This was an important breakthrough as the energy density of supercapacitors, relatively low compared to batteries, is what currently limits their application. The progress towards more powerful supercapacitors is limited by our incomplete understanding of the relation between their performance, in particular their capacitance and charging rate, and the complex structure of the porous carbon electrodes. To make progress we need a better fundamental understanding of the ion transport and electrolyte structure in the pores. In this project we are planning to use classical molecular dynamics simulations to calculate the capacitive and transport properties of a range of systems. We will focus on model ordered three-dimensional porous carbons which are currently the missing link between oversimplified geometries, such as planar graphitic structures and carbon nanotubes, and disordered realistic structures. This will allow us to vary geometric descriptors, e.g. pore size and ion size, in a systematic way and obtain relevant microscopic information. This classical molecular dynamics study will be coupled with the development of original mesoscopic models in order to allow for a systematic screening of porous carbons for energy storage application.

Dernières publications:

- On the development of an original mesoscopic model to predict the capacitive properties of carbon-carbon supercapacitors, A. Belhboub, E. H. Lahrar, P. Simon and C. Merlet, Electrochim. Acta, 327, 135022 (2019) - **doi:** pu.doi **url:** pu.open_url
- Ionic liquids under confinement: From systematic variations of the ion and pore sizes towards an understanding of structure and dynamics in complex porous carbons, ACS Applied Materials & Interfaces, just accepted - **doi:** pu.doi

Méthodes stochastiques pour l'exploration du paysage énergétique de systèmes moléculaires : Application aux biomolécules sur surfaces

Projet démarré en 2016

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Nathalie Tarrat**

Comprendre la structure et le comportement des biomolécules sur des surfaces est d'un grand intérêt pour la recherche fondamentale et les applications technologiques. Ces dernières années, des algorithmes issus de la recherche en robotique sont apparus comme une nouvelle approche pour l'exploration du paysage énergétique

de systèmes moléculaires. En collaboration MPI (Stuttgart, Allemagne) et l'université de Koskalin (Pologne), nous appliquons ces méthodes à l'étude de disaccharides sur des surfaces métalliques. Notre projet consiste à identifier un ensemble de conformations correspondant aux états les plus probables du système. Etant donné que les états les plus probables sont ceux qui minimisent l'énergie du système, il s'agit donc de résoudre un problème d'optimisation globale, dans lequel il ne s'agit pas de calculer seulement le minimum global, mais un ensemble de minima suffisamment représentatif. Pour traiter ce problème en très haute dimension, nous travaillons au couplage de méthodes stochastiques d'exploration et d'échantillonnage inspirées d'algorithmes utilisés en robotique avec des méthodes d'optimisation locale et des méthodes de clustering. Après avoir paramétré et validé notre modèle atomistique, nous avons focalisé notre première étude sur l'auto-organisation de deux sucres (tréhalose et sucrose) sur une surface de métallique, Cu(100), systèmes pour lesquels nous disposions de données expérimentales (images STM réalisées au MPI). Pour cela, nous avons mis au point un protocole multi-échelle nous permettant d'aller de l'étude de la molécule unique, validée au préalable sur le trehalose, à la simulation des images STM de sucres auto-organisés. Nous avons pu proposer des modèles d'auto-organisation compatibles avec les images expérimentales. L'étape suivante de notre projet consiste à étudier les différences de réactivité vis-à-vis d'un disaccharide (lactose) des différentes facettes cristallographiques du cuivre, de l'or et de l'argent. En 2018, nous avons étudié l'adsorption du lactose dans sa conformation chaise sur les surfaces Cu(100), Cu(110) et Cu(111). La suite de ce travail, i.e. l'étude de l'adsorption du lactose sur l'argent et l'or fait l'objet de notre demande de ressources 2019. Nous souhaitons également réaliser en 2019 des trajectoires de dynamique moléculaire afin de nous assurer que les cycles galactose et glucose formant le lactose demeurent en conformation chaise à haute température lorsqu'ils sont déposés sur la surface.

Dernières publications:

- Angewandte Chemie Int. Ed., 2019, 58, 8336. - **doi:** pu.doi
- RSC Advances, 2019, 9, 35813 - 35819 - **doi:** pu.doi

Interprétation atomistique du fonctionnement d'un capteur de gaz

Projet démarré en 2016

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Anne Hemeryck**

Water vapour is the omnipresent interfering component for gas sensing in ambient conditions. Even more than four decades after the first SMOX-based gas sensor came on the market, the cross sensitivity to water vapour is still one of big issues for gas sensing in ambient conditions. Most of the current models describing the interaction of water vapour with SMOX surface were empirically developed more than one or two decades ago and fail to satisfactory explain the recent experimental findings. A critical revision based on modern theoretical calculations seems to be inevitable. DFT calculations approach is considered to be a powerful approach to understand the surface reactions on an atomistic level, determining involved surface species and their influence on the electronic structure of the solid. This project is developed in the frame of a collaboration between the LAAS from Toulouse and the University of Tuebingen in Germany. Several metal oxides materials are under study, namely SnO2, WO3 and In2O3. The goal of this project is to get a detailed picture of the reaction of gas molecule (CO, CO2, H2, N2, NO2...) on clean and defective surfaces of the metal oxides, and also to understand how humidity can affect the detection process. The study of water effect is thus performed on SnO2, WO3 and In2O3 surfaces. The concentration and type of defects such as bulk/surface oxygen vacancies or surface hydroxyl groups will be considered.

Dernières publications:

- Ambient humidity influence of CO detection with SnO2 gas sensing materials - a DRIFTS/DFT investigation - Susanne Wicker, Mathilde Guiltat, Udo Weimar, Anne Hemeryck, Nicolae Barsan, Journal of Physical Chemistry C 121 (2017) 25064–25073 - **doi:** pu.doi **url:** pu.open_url

Effets de déplacement atomique dans le silicium pour le durcissement des capteurs CMOS

Projet démarré en 2015

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Anne Hemeryck**

Today, the development of new experimental facilities surrounded by a nuclear environment is accompanied by a need for resistant systems to radiation, so-called "hardened" for diagnostics and security. The improvement and adaptation of the holding of these systems to these extreme environments can be achieved through the adaptation of their architecture. However, it appears essential to help the hardening of the component thanks to a better knowledge of the physical phenomena of degradation under irradiation taking place in the material layers constituting component. This is particularly the case for the new generation of imagers based on CMOS sensors (for "Complementary Metal Oxide Semiconductor"). These are planned to replace CCDs (for "Charge-Coupled Device") in nuclear installations. Therefore, a multi-levels study dedicated to the understanding of the formation of defects and the effects of these atomic displacements due to radiation in silicon constituting CMOS sensors is set up using Dynamic Molecular technique, kinetic Activation Relaxation Technique and ab initio calculations. The current step of calculations concerns ab initio characterizations of the permanent formed defects using LDA methodology and GW methodology, then those data will be used to establish the link with the experimental DC-Random-Telegraph-Signals in macroscopic models. Now the modeling approach is validated, we expect to draw a complete, detailed and well-characterized list of all kind of defects that can exist in embedded devices such as Si-based and Ge-based devices.

Dernières publications:

- Simulation of Single Particle Displacement Damage in Silicon – Part II: Generation and Long-Time Relaxation of Damage Structure - Antoine Jay, Mélanie Raine, Nicolas Richard, Normand Mousseau, Vincent Goiffon, Anne Hémeryck, Pierre Magnan - IEEE Transactions on Nuclear Science 64 (2017) 141-148 - **doi:** pu.doi
- Simulation of Single Particle Displacement Damage in Silicon – Part III: Generation and Long-Time Relaxation of Damage Structure - Antoine Jay, Anne Hémeryck, Nicolas Richard, Layla Martin Samos, Mélanie Raine, Alexandre Le Roch, Normand Mousseau, Vincent Goiffon, Philippe Paillet, Marc Gaillardin, Pierre Magnan - IEEE Transactions on Nuclear Science 65 (2018) 724-731 - **doi:** pu.doi

Heudyn

Projet démarré en 2015

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Nicolas Biziere**

The Heudyn project aims at calculating the spin waves frequencies in magnonic crystals made of Co2MnSi alloys. To achieve this goal, we perform micromagnetic simulations in time domain from a quasistatic equilibrium position of the magnetization. The calculation is performed in cubic cells and the results of the time varying magnetization position is recorded for FFT post-treatment revealing the spin waves amplitudes and frequencies in the magnonic crystal. The results of this calculation are compared to experimental measurements realized at the CEMES lab. The spin wave measurement are performed on millimeters samples in microstrip configurations

up to 30 GHz. The size of the simulated samples must avoid artefacts in the determination of the stationary modes such as reflection of spin waves on the edge of the sample. Then we want to simulate the dynamic magnetic states of big samples composed of few millions of nanometric cells.

Dernières publications:

- Multi magnetic states in Co/Cu multilayered cylindrical nanowires studied by combination of off-axis electron holography imaging and micromagnetic simulations. N. Biziere, D. Reyes, T. L. Wade, B. Warot-Fonrose and C. Gatel,, J. Appl. Phys. 126, 163906, 2019. - **doi:** pu.doi
- Holographic Vector Field Electron Tomography of Three-Dimensional Nanomagnets, Daniel Wolf, Nicolas Biziere, Sebastian Sturm, David Reyes, Travis Wade, Tore Niermann, Jonas Krehl, Bénédicte Warot-Fonrose, Bernd Büchner, Etienne Snoeck, Christophe Gatel, and Axel Lubk, Communications Physics, 2, 87, 2019. - **doi:** pu.doi

Representative models of polymer surfaces using MD and DFT studies: poly-epoxy and organosilicates surfaces

Projet démarré en 2015

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)

Porteur de projet: **Corinne Dufaure**

The aim of our project is to construct models of polymer surfaces and to simulate XPS spectra of the surfaces to validate our computational approach by comparison with experimental XPS spectra. We work on two polymers, i.e. poly-epoxy polymers and organisilicates polymers. In order to investigate the model surface reactivity of poly-epoxies, a polymerized mixture of bisphenol A diglycidyl ether (DGEBA) and ethylenediamine (EDA), DFT and MD calculations were used. We first chose a dimer model (DGEBA + EDA) in order to compute XPS core-level shifts using DFT calculations. Simulated XPS spectra for the pristine and metallized surfaces compared well with experimental counterpart, leading to a more accurate interpretation of the experimental spectrum than with the exclusive use of literature. DFT calculations were also performed to study the first step of the metallization process, i.e. adsorption of Cu atoms on the polymer model surface. We concluded that the adsorption on the hydroxyl groups of the polymer is favored. In addition, MD simulations were performed to get a more realistic model and the thermal and volumetric properties of the model poly-epoxy were also characterized by the determination of the density, the coefficient of volumic thermal expansion and the glass transition temperature Tg of the polymer and the comparison with available experimental data. We created a bulk polymer and we want now to create a polymer surface using the same procedure. We also want to design models for the surface of organosilicate membranes to study the sorption of the different interacting species.

Dernières publications:

- A. Gavrielides, T. Duguet, M. Aufray, C. Lacaze-Dufaure, Model of the DGEBA-EDA epoxy polymer: experiments and simulation using classical molecular dynamics, International Journal of Polymer Science, International Journal of polymer Science, p.9604714 (2019). -
- T. Duguet, A. Gavrielides, J. Esvan, T. Mineva, C. Lacaze-Dufaure, DFT Simulation of XPS Reveals Cu / Epoxy Polymer Interfacial Bonding, The Journal of Physical Chemistry C, accepted -

Calcul ab initio de spectres XANES et EELS pour l'interprétation de spectres expérimentaux.

Projet démarré en 2015

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Benedicte Warot-Fonrose**

In this project, we propose to use DFT-based first principles methods to calculate the electron energy loss spectra (EELS) and/or the X-ray absorption near-edge structures spectra (XANES) of different kinds of oxides potentially very important for technological applications. These calculations will be very helpful for experimentalists (in particular those working at the CEMES) to interpret experimental spectra in terms of the local electronic structure. Used as finger prints, the calculated spectra will also help experimentalists identifying crystal phases in complex samples, when nanocrystals are too small for being studied individually with conventional diffraction techniques and when experimental spectra recorded on reference crystals are not available. We will in particular calculate oxygen K-edge EELS spectra in complex oxides potentially strongly interesting for electronic and spintronic applications (half-metals, ferroelectrics or multiferroics). A comparison of the spectra obtained with different DFT-based codes and with different methods will be performed.

Dernières publications:

- M. Lee, R. Arras, B. Warot-Fonrose, T. Hungria, M. Lippmaa, H. Daimon and M. J. Casanove, Phys. Chem. Chem. Phys. 19, 28676 (2017). - **doi:** pu.doi
- M. Lee, R. Arras, R. Takahashi, B. Warot-Fonrose, H. Daimon, M.-J. Casanove, M. Lippmaa, ACS Omega 3, 2169 (2018). - **doi:** pu.doi

STRUCTURE ELECTRONIQUE ET INJECTION DE SPINDANS LES JONCTIONS METAL FERROMAGNETIQUE/ISOLANT/SEMICONDUCTEUR

Projet démarré en 2014

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Lionel Calmels**

CE PROJET A ETE SOUMIS CETTE ANNEE A UN APPEL D'OFFRE EN VUE D'OBTENIR LE COFINANCEMENT D'UNE THESE PAR LA REGION MIDI-PYRENEES ET LE PRES. NOUS VENONS D'APPRENDRE QUE NOTRE PROJET A ETE SELECTIONNE. UN DOCTORANT DEVRAIT DONC ARRIVER A L'AUTOMNE POUR TRAVAILLER SUR CE PROJET. Cette thèse sera centrée sur l'étude théorique des états électroniques de multicouches permettant l'injection de spin dans des semiconducteurs. Les fonctions d'onde décrivant le comportement des électrons seront calculées au CEMES par des méthodes ab-initio, avec des codes déjà existants basés sur la théorie de la fonctionnelle de la densité (DFT), tels que les codes Wien2k et VASP. Ces codes permettent de décrire le raccordement des fonctions d'onde aux interfaces de la multicouche, en fonction de leur structure atomique. Les multicouches qui seront étudiées sont les jonctions CoFeB (ou Fe)/MgO/GaAs(001), ainsi que des multicouches à base de semiconducteurs bidimensionnels (domaine de recherche en plein essor à l'heure actuelle) tels que MoS2, WS2, WSe2. Ces calculs devraient être très lourds (plusieurs interfaces dans le même système, un grand nombre d'atomes à prendre en compte). C'est pourquoi nous avons besoin de 250000 heures pour le lancer (automne/hiver 2014).

Dernières publications:

- Spin-Polarized Electron Tunneling in bcc FeCo/MgO/FeCo(001) Magnetic Tunnel Junctions -
- Half-metallicity, magnetic moments, and gap states in oxygen-deficient magnetite for spintronic applications -

Compréhension des mécanismes de croissance des matériaux et de formation des interfaces

Projet démarré en 2014

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Anne Hemeryck**

The overall aim of this project is help technological development toward the integration of ultra-thin and nanoscale mastered oxide layers in the context of Microelectronics. These integrated materials must be now characterized by tailored structural and electronic properties, achievable thanks to the control of the atomic arrangement. The main objective of this project is to push forward these developments through a fundamental understanding of the local mechanisms involved during the growth of integrated materials. We want to provide models required by technologists in order to master the steps of deposition process of metal oxides layers as a function of the applied technological process. In fine, our challenge is to be able to provide a macroscopic model as TCAD tool dedicated to the deposition process simulation (based on kinetic Monte Carlo methodology where DFT data are used as input parameters). In order to provide a multi-processes, multi-materials simulation platform, this project is developed on two main materials: - Simulating the growth of Si/SiO2 interface as a thermal oxidation process thanks to the ARTn/VASP coupling developed by A. Hemeryck and coworkers to propose an ab initio Si/SiO2 interface model - Growth of Bi nanowires on Silicium substrates using DFT calculations

Dernières publications:

- Modeling Of The Interface Formation During CuO Deposition On Al(111) Substrate: Linking Material Design and Elaboration Process Parameters Through Multi-Levels Approach - Mathilde Guiltat, Nicolas Salles, Marie Brut, Georges Landa,Nicolas Richard, Sébastien Vizzini, Anne Hémeryck - Modelling and Simulation in Materials Science and Engineering 25 (2017) 064005 - **doi:** pu.doi
- Insight of Surfaces Treatments for CMOS Compatibility of InAs Nanowires - Daya Dhungana, Anne Hemeryck, Nicolo Sartori, Pier-Francesco Fazzini, Fuccio Cristiano, Sébastien Plissard - Nano Research 12 (2019) 581–586 - **doi:** pu.doi **url:** pu.open_url

Simulation du torque généré par des assemblées de nanoparticules magnétiques en interaction.

Projet démarré en 2014

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Julian Carrey**

We have developed a kinetic Monte-Carlo program which is able to simulate the torque properties of an assembly of magnetic nanoparticles in interactions, and published a first theoretical article on this subject. Next year, we would like to focus on a new problem : the influence of a static magnetic field on the torque properties of an assembly of magnetic nanoparticles. This study is important for biological applications for two reasons. First, if a static magnetic field can improve the torque properties of the assembly, it could be easily implemented experimentally: a permanent magnet could be added to setups generating rotating magnetic fields, and the effect on the cellular death studied. Second, in case a static magnetic field is able to decrease strongly the torque amplitude, this effect could be used to localize cellular death in specific parts of the body (for instance in the tumor only). This would be possible by adding gradient field coils to the setup generating the rotating magnetic field, so that there is a point in the space – the position of which can be controlled – where the static magnetic field is null: cellular death would occur only around this point. This work will require to use a program which is already written and will thus not require new software development. We estimate that 30000 hours should permit to achieve this objective.

Dernières publications:

- J. Carrey and N. Hallali, Phys. Rev. B 94, 184420 (2016) - **doi:** pu.doi
- J. Carrey and N. Hallali, Phys. Rev. B 98, 139902(E) (2018) - **doi:** pu.doi

Modélisation et optimisation de nanoparticules métalliques bactéricides

Projet démarré en 2013

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Nathalie Tarrat**

L'objectif de ce projet est d'étudier les liens entre la morphologie d'une nanoparticule d'or et sa capacité d'adsorption de molécules antibactériennes en surface. Afin d'étudier ces systèmes, nous travaillons à l'adaptation d'une méthode approximée, la SCC-DFTB. En effet, cette dernière nous permettra d'étudier des systèmes très étendus comprenant la nanoparticule et son environnement organique avec une précision proche de celle des calculs DFT mais avec un coût calculatoire bien moindre. Afin d'acquérir une compréhension précise de l'interface nanoparticule d'or / (bio)-molécule et de générer un jeu de données permettant de tester la validité de cette méthode quasi quantique, nous avons réalisé ces dernières années des études DFT sur des modèles de surfaces d'or fonctionnalisées par des antibiotiques ou par des groupements modèles. Ce travail nous a permis de démontrer le rôle crucial joué par les interactions inter-moléculaires dans la stabilisation des systèmes hybrides « nanoparticules-antibiotiques » ainsi que d'aller plus en avant dans la compréhension des rôles joués par les différents groupements chimiques des antibiotiques dans le phénomène d'adsorption sur l'or. Concernant le développement des paramètres DFTB, nous avons pour l'instant validé la performance de nos paramètres vis-à-vis de la modélisation de nanoparticules d'or dans le vide et en solution aqueuse. Ces développements nous ont déjà permis de réaliser des explorations structurales de nanoparticules et de calculer des propriétés thermodynamiques d'agrégats métalliques jusque-là très difficilement accessibles avec un si haut niveau de théorie. Nous avons mis en lumière la structuration originale de nanoparticules d'or dans la gamme Au55-147: apparition de cavités ou organisation de type cœur-coquille (cœur désordonné et surface régulière). De plus, nous avons montré sur Au20 que, bien que la variation de la charge (0, + 1, -1) ne modifie pas la structure d'équilibre pyramidale, elle affecte fortement la température de fusion. La suite de notre projet va consister à tester la performance de nos paramètres DFTB vis-à-vis de la description des différentes facettes cristallographiques de l'or susceptibles d'être exposées à la surface des nanoparticules d'or, Au(111), Au(100) et Au(110). Seront calculées les énergies de surface, les distances interplanaires, et le travail de sortie pour chaque type de surface et ces données seront comparées aux données expérimentales et aux données DFT. Une fois ce travail réalisé, nous optimiserons les paramètres DFTB décrivant l'interaction surface d'or-antibiotiques et ces derniers seront testés par comparaison avec notre banque de données DFT établie sur les groupements modèles (S-CH3, O-CH3, NH-CH3) adsorbés sur les 3 facettes d'or.

Dernières publications:

- Materialia, 2018, 4, 297 - **doi:** pu.doi
- Phys. Chem. Chem. Phys., , 2019, 21, 24857. - **doi:** pu.doi

Anisotropie magnétique des couches minces et multicouches pour l'électronique de spin

Projet démarré en 2012

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Etienne Snoeck**

This project consists in calculating the magnetic anisotropy energy of several kinds of magnetic multilayers which are interesting for their potential application in spintronic devices. We will calculate the anisotropy energy of crystals in which the magnetic anisotropy is strongly enhanced by interfaces between magnetic and non-magnetic materials. The magnetic materials which will be sudied here are: - thin Fe layers grown on the top of a non magnetic bcc substrate - thin layers of full Heusler alloys such as Co2MnSi, Co2FeSi, Co2FeAl, Co2Fe(Al,Si)which will be sandwiched between non magnetic metals such as Pt and Pd. We will calculate which thicknesses and which interfaces must be chosen to reach a magnetic anisotropy perpendicular to the interfaces. The magnetic

anisotropy of these multilayers will be interpreted in terms of the electronic structure, starting from the perturbation theory which describes the modification of the ground state energy induced by spin-orbit coupling: the electron states responsible for the perpendicular anisotropy will be either degenerated states near the Fermi level (they contribute at the first order perturbation theory), or occupied and unoccupied non degenerated states (they contribute at the second order perturbation theory).

Dernières publications:

- PHYSICAL REVIEW B 90, 45411 (2014) -
- JOURNAL OF PHYSICS-CONDENSED MATTER 25, 256002 (2013) -

ETUDES NUMERIQUES DE SYSTÈMES FORTEMENT CORRELES EN MATIERE CONDENSEE OU DANS LES SYSTEMES D'ATOMES ULTRA-FROIDS SUR RESEAUX

Projet démarré en 2012

LPT - Laboratoire de Physique Théorique (UMR 5152)

Porteur de projet: **Didier Poilblanc**

The scientific activity briefly described here is directly connected to the most active domains of research in the field of correlated systems such as unconventional and high-Tc superconductors, quantum phase transitions, low-dimensional conductors, novel fractional quantum Hall states and emerging non-Abelian excitations, ultra-cold atoms loaded on optical traps, entanglement & quantum information, etc. Our activity is two-fold: (i) using well optimized numerical methods (such as home-made Lanczos exact diagonalisation, Density Matrix Renormalization Group algorithm or variational quantum Monte Carlo algorithm) to tackle models of correlated systems and achieve the best refined comparison with many of the related experimental systems and (ii) develop new numerical methods like tensor network techniques borrowing novel concepts from quantum information to be able to address larger systems, still with a very good accuracy.

Dernières publications:

- Gapped Z2 spin liquid in the breathing kagome Heisenberg antiferromagnet, Mohsin Iqbal, Didier Poilblanc, Norbert Schuch, submitted to Phys. Rev. B. -
- Quantum spin liquid phases in the bilinear-biquadratic two-SU(4)-fermion Hamiltonian on the square lattice, O. Gauthé, S. Capponi, M. Mambrini and D. Poilblanc, in preparation. -

Gaz bidimensionnel d'électrons aux interfaces tout-oxydes

Projet démarré en 2012

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Rémi Arras**

This project will focuse on the study of oxide-based heterostructures, at the interfaces of which an intrinsic and (fully-spin polarized) electron gas can be stabilized. Such system is of great interests for designing new electronic and spintronic devices, like (spin-)FET.

Dernières publications:

- M. J. Veit, M. K. Chan, B. J. Ramshaw, R. Arras, R. Pentcheva, and Y. Suzuki, Phys. Rev. B 99, 115126 (2019). - **doi:** pu.doi
- R. Arras and S. Cherifi-Hertel, ACS Appl. Mater. Interfaces 11, 34399 (2019) - **doi:** pu.doi

DFT STUDIES OF THE INHIBITION OF THE CORROSION OF ALUMINUM AND OXIDES

Projet démarré en 2012

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)

Porteur de projet: **Corinne Dufaure**

Recently, the high toxicity of chromates has imposed restrictions on their use in industrial applications. It is mandatory to find new environmentally friendly compounds as corrosion inhibitors of aluminum and aluminum alloys. This project aims to investigate, at the atomic scale, the corrosion inhibition mechanisms affecting aluminum. We propose to determine the mode of action of an efficient corrosion inhibitor by using ab initio calculation. In the past years, we studied the interaction of the 8-hydroxyquinoline (8HQ) and derivatives with aluminum surfaces with a periodic/DFT-D approach. We also investigated the reactivity towards molecular oxygen of the organic layers adsorbed on Al(111). O2 dissociation was not observed on the most compact layers. In addition, we studied the adsorption of the 8HQ molecule on hydroxylated aluminum oxide. The chemisorption of the organic molecules led to an electronic redistribution in the systems that could change the surface reactivity. In order to demonstrate it, we want now to investigate the interaction of molecular oxygen with the oxide covered by the organic layer. We now study a set of organics inhibitors analogues to 8-HQ but showing no corrosion inhibition efficiency. We perform DFT computations on the isolated molecules but also on Al complexes in order to determine energetic, structural, electronic, topological… descriptors in relation with corrosion inhibition. We expect that all these ab initio calculations will give insights in the relation between the chemical nature of the surface, the chemical structure of the inhibitor, the inhibitors/surface interactions and the inhibition efficiency of a molecule. It will help us to rationalize the search of alternative inhibiting species against the corrosion of aluminum and its alloys.

Dernières publications:

- Surface Science 2011, 605, 341 -
- F. Chiter, M-L. Bonnet, C. Lacaze-Dufaure, H. Tang and N. Pébère, Phys. Chem. Chem. Phys., 20 (2018) 21474. -

Mobilités des joints de grain sous contrainte

Projet démarré en 2012

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Nicolas Combe**

Structural materials with nanoscritalline grains (<100nm) are very promising due to their very good mechanical properties. These mechanical properties are noticeably related to the mobility of grain boundaries (GB). The present project proposes to study homogeneous nucleation of disconnection in Aluminum grain boundaries and the inhomogenous nucleation of disconnections resulting from the absorption of bulk dislocations in copper. The structural and energetic study of the GB migration will be studied using the Nudge Elastic band method between two states corresponding to the positions of the GB before and after the migration. In addition, the calculation of the free energy of the migration as a function of a collective variables will be performed using the Adaptive Biasing Forces and the metadynamic method.

Dernières publications:

- Phys. Rev. Mat., 1, 033605 (2017) - **doi:** pu.doi
- Phys. Rev. Materials, 3 , 060601, (2019) - **doi:** pu.doi

Linear and nonlinear optical properties of high refractive index dielectric nanostructuress: A numerical study

Projet démarré en 2012

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Vincent Paillard**

Compared to the bulk material, semiconductor nanostructures exhibit enhanced absorption and scattering efficiencies. These properties can be theoretically predicted for spherical or cylindrical particles by the analytical Lorenz-Mie theory for non-absorbing, homogeneous environments. To determine deviations from this ideal case (finite length, presence of a substrate, non-circular shape …), approximative numerical methods must be used such as the Green Dyadic method (GDM). Recently we focused on nonlinear effects in Silicon nanowires, in particular the experimental observation of an intense polarization-dependent Second Harmonic Generation (SHG), normally forbidden in bulk silicon. As in other centrosymmetric nanostructures such as gold nanorods and nanoparticles, there are different electric dipolar (surface) and higher order (volume) contributions to SHG. We developed code to calculate the possible contributions to SHG from centrosymmetric media. Thanks to extensive numerical simulations we found a transition between a field-gradient induced bulk- and a local surface contribution to SHG. These sources can be individually addressed by simply changing the polarization state of the illuminating fundamental light, or by varying the nanowire diameter. In a second project, we coupled the GDM to evolutionary optimization algorithms, capable to target multiple optimization objectives simultaneously. Thanks to this, we are able to automatically design double-resonant nanostructures, having polarization dependent, individually addressable resonances at arbitrary, user-specific wavelengths. The method allows other optimization targets as well. Recently, we furthermore demonstrated that also complex properties such as the decay-rate of electric or magnetic dipole emitters close to a nanostructure or thermoplasmonic effects (strongly localized, optical heating at the nano-scale) can be tailored using evolutionary optimization. Most recently, we started working on applications of deep learning for nano-photonics. We demonstrated that optical information storage with bit-densities well beyond the optical diffraction limit can be enabled by using a machine learning driven read-out scheme.

Dernières publications:

- C. Majorel, V. Paillard, A. Patoux, P. R. Wiecha, A. Cuche, A. Arbouet, C. Bonafos, C. Girard, "Theory of plasmonic properties of hyper-doped silicon nanostructures," Optics communications, vol. 453 (2019). - **doi:** pu.doi
- P. R. Wiecha, C. Majorel, C. Girard, A. Arbouet, B. Masenelli, O. Boisron, A. Lecestre, G. Larrieu, A. Cuche, V. Paillard, Tailoring electric and magnetic dipole emissions by high-refractive index dielectric nanostructures. META 2019, Symp. I "Hybrid photonic and plasmonic materails for sensing, energy conversion and imaging applications", Lisbon, Portugal, July 24-27, 2019. Invited Talk - **doi:** pu.doi

Étude de nanoparticules cœur-coquille Fe@Au

Projet démarré en 2011

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Magali BENOIT**

Bimetallic nanoparticles are of great interest due the effect of the reduced size on their properties but also due to the effect of the chemistry of the system. The chemical composition inside the particle is a very important parameter with respect to the properties. Au-Fe nanoparticles have potential applications in catalysis and bio-medicine. It is therefore fundamental to know their morphology, which can be controlled by the growth

parameters. Experimentalists at CEMES have elaborated Au-Fe nanoparticles with a Fe core and an Au shell. The epitaxial relationships have been studied by transmission electronic microscopy. In order to understand the formation mechanism of these particles, in 2012 and 2014, we have studied the Au(001)/Fe(001) interface, using spin-polarized DFT calculations in the GGA approximation, and have extracted the interface energy from these calculations. In 2016, we have shown that Fe@Au nanoparticles may have different surface reactivity depending on the number of gold layers in the Au shell. Finally, in 2017, we have developed a new Fe-Au EAM potential that we have started to use for large-scale molecular dynamics and Monte Carlo simulations. In 2018, we have started the study of the growth mechanisms during gold deposition and its impact on the morphology of these nanoparticles. In 2019, we will continue these studies and analyze the transition between the Wulff to cube morphology of the Fe core.

Dernières publications:

- P. Benzo, M. Benoit, N. Tarrat, C. Langlois, R. Arenal, B. P\'ecassou, A. Le Priol, N. Combe, A. Ponchet and M.-J. Casanove, IEEE Nanotechnology Materials and Devices Conference (NMDC) (2017) -
- C. Langlois, M. Benoit, J. Nicolai, N. Combe, R. Arenal, A. Ponchet, and M.-J. Casanove, Nano Letters 15, 5075 (2015) -

Modelisation du depot et de l'initiation de materiaux energetiques nano-structures de type thermite

Projet démarré en 2010

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Alain Esteve**

Energetic materials have attracted a growing interest these last years due to their capability to provide on-board energy. Within this context LAAS experimentalists are developing new techniques for integrating Al/CuO thermite in pyrotechnic microsystems. However, the properties of thermites are not well understood neither from the synthesis nor their thermal characteristics. Therefore, we use multi-scale calculations in order to gain a better understanding involved during the deposition and initiation processes in order to build a meso- or macroscopic model for guiding experimentalists in the design of ad-hoc materials.

Dernières publications:

- Al Interaction with ZnO Surfaces Yuzhi Gao, Mathilde Iachella, Eric Mattson, Antonio T. Lucero, Jiyoung Kim, Mehdi Djafari Rouhani, Yves Chabal, Carole Rossi, Alain Estève ACS J. Phys. Chem. C 122 (31), 17856, -
- Al Interaction with ZnO Surfaces Yuzhi Gao, Mathilde Iachella, Eric Mattson, Antonio T. Lucero, Jiyoung Kim, Mehdi Djafari Rouhani, Yves Chabal, Carole Rossi, Alain Estève ACS J. Phys. Chem. C 122 (31), 17856, -

Simulation des propriétés optiques de nano-objets et nanostructures métalliques.

Projet démarré en 2009

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Adnen Mlayah**

Les nano-objets et nanostructures métalliques absorbent, diffusent, transmettent et guident la lumière dans une gamme de longueur d'onde qui s'étale du proche UV (0.3 nm) jusqu'à l'infrarouge lointain (3 µm) grâce à l'excitation optique d'oscillations collectives de leurs électrons libres, les plasmons de surface. De plus, leur taille nanométrique et le grand rapport surface/volume leur confèrent la capacité de localiser spatialement l'énergie

électromagnétique. De ces propriétés découlent des applications dans des domaines aussi variés que ceux des télécommunications, de la production d'énergie, des capteurs chimiques et biologiques, du diagnostic et de la thérapie en cancérologie. La simulation/modélisation des propriétés optiques de nano-objets métalliques est un outil non seulement d'interprétation des expériences de spectroscopies optiques (absorption,luminescence, Rayleigh-Mie, Raman-Brillouiun, Luminescence à deux photons) mais aussi de "design" de la nature, de la taille, de la forme des nano-objets visant une propriété optique particulière (exaltation de l'émission, guidage optique, hyperthermie). Le projet présenté ici s'inscrit dans cette thématique de recherche "plasmonique". Il vise l'utilisation de techniques de simulations numériques des spectres d'extinction et d'absorption optique et du champ proche électromagnetique au voisinage des surfaces de nano-objets métalliques. Le projet s'inscrit dans le cadre des activités "plasmonique" du CEMES, axe transversal au sein du laboratoire. Ce projet fait l'objet de collaborations internationales (Institute for Material Research and Engeneering/ Singapore, Donostia International Physics Center de San Sebastian; Rice University, Houston, UTSA San Antonio) qui se poursuivent.

Dernières publications:

- Temperature dependent plasmon-exciton interation in hybrid MoSe2/Au nanostructures Inès Abid, Weibing Chen, Jiangtan Yuan, Arash Bohloul, Sina Najmaei, Carolina Avendano, Renaud Péchou, Adnen Mlayah and Jun Lou ACS Photonics 2017, 4, 1653−1660 - **doi:** pu.doi
- Resonant Surface Enhanced Raman Scattering in Hybrid MoSe2/Au Nanostructures Inès Abid, Weibing Chen, Jiangtan Yuan, Arash Bohloul, Sina Najmaei, Carolina Avendano, Renaud Péchou, Adnen Mlayah and Jun Lou Optics Express, Vol. 26, Issue 22, pp. 29411-29423 - **doi:** pu.doi

Etude par DFT des nanorods FeS2 comme matéraiux pour cathode dans les batteries sodium-ion.

Projet démarré en 2009

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Hao Tang**

The iron disulfide FeS2 is one of the most abundant minerals present in nature. The most popular crystallin forms are the Pyrite (also called Fool's Good) and the Marcasite. Even already used by the ancient Greek, it became attractive again thanks to many interessting properties for applications as catalyst for water splitting, photovoltaic devices [2] and cathode for Lithium ion battery and sodium ion battery [3]. The sodium ion batteries (SIBs) are considered as a serious candidate for energy storage in mobility in large use area due to the abundance of raw materials. The performance of SIBs could be improved by using ultrafine iron pyrite (FeS2) nanocrystals as electrodes materials [3]. However, the mechanism involved in such improvement is still unknow. In this project, we are aiming on studying by DFT the interaction of sodium ions with nanocrystallin pyrite, in order to find possible explaination of this performance.

Dernières publications:

- "Magnetism and morphology in facetedB2-ordered FeRh nanoparticles", M. Liu, P. Benzo, H. Tang, M. Castiella, B. Warot-Fonrose, N. Tarrat, C. Gatel, M. Respaud, J. Morillo and M. J. Casanove, Eur. Phys. Lett., 116, 27006 (2016). - **url:** pu.open_url
- "Prediction of Co nanopareticle morphologies stabilized by ligands : towards a kinetic model", Van Bac Hguyen, M. Benoit, N. Come and H. Tang , Phys. Chem. Chem. Phys., 19, 4636-4647 (2017). - **url:** pu.open_url

Étude de la solubilité et de la diffusion de l'oxygène dans les superalliages à base de nickel

Projet démarré en 2009

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)

Porteur de projet: **Damien Connétable**

In the context of lifetime prediction of numerous industrial devices working at high temperature and oxidizing atmospheres (heat converter in nuclear power plants, solar hoven, gaz turbines, …). we propose to study the mechanisms involved in high temperature oxidation of nickel-based superalloys which result in the formation of cavities in the substrate. The project will involve both, numerical studies by the mean of atomistic simulations together with a mesoscopic model and experimental studies on model materials. The project is focused on the formation of cavities in the substrate, that are observed during high temperature oxidation of nickel-based superalloys, and the diffusion of the O atoms in the substrat and its interactions with others defects.

Dernières publications:

- "Elastic properties of the α' martensitic phase of the Ti-6Al-4V alloys obtained by additive manufacturing." N. Dumonet, D. Connétable, B. Viguier and B. Malard, Scripta Materialia 167 (2019) 115-119. - **url:** pu.open_url
- Stress-controlled carbon diffusion channeling in bct- iron: a mean-field theory.'', P. Maugis, S. Chentouf and D. Connétable Journal of Alloys and Compounds 769 (2018) 1121-1131. - **url:** pu.open_url

Structure électronique des matériaux d'électrodes pour jonctions tunnel magnétiques Métal/MgO/Métal

Projet démarré en 2008

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Lionel Calmels**

Les calculs que nous souhaitons mener au cours des prochaines années permettront de comprendre la structure électronique des jonctions tunnel magnétiques dont les électrodes sont constituées de métaux 3d (essentiellement le fer et le cobalt). Il s\'agira également de calculer les spectres EELS permettant de faire des mesures locales de cette structure électronique afin de comprendre et interpréter les résultats des mesures expérimentales menées sur ces systèmes. •Calcul de la structure électronique des jonctions « Métal 3d/MgO/Métal 3d »: Le but de notre projet est de comprendre les mécanismes de transport dans les jonctions tunnel ainsi que la connection entre les propriétés de magnétotransport et le couplage magnétique entre les deux électrodes. En l'absence de polarisation et pour des jonctions peu épaisses avec des interfaces parfaitement planes, le couplage n'est pas dû aux interactions dipolaires de type "peau d'orange" mais aux électrons qui traversent la jonction par effet tunnel, dans les deux sens et avec un courant résultant nul. Les calculs de structure électronique permettront de comprendre comment les fonctions d'onde se comportent aux interfaces de la barrière et au travers de celle-ci lorsqu'on modifie la nature des électrodes magnétiques et des interfaces. Une première série de calculs portera sur la jonction Co(hcp)/MgO/Co(hcp). La structure atomique de cette jonction est telle que l'axe c du cobalt est couché dans le plan de croissance et la fine barrière de MgO est contrainte sur le cobalt. La structure atomique (hcp) des électrodes magnétiques et des interfaces de cette jonction est différente de celle des jonctions à électrodes bcc qui ont jusqu'à présent été abondamment étudiées. Ces calculs vont permettre de comprendre comment des états électroniques ayant une symétrie autre que celles des électrodes bcc peuvent être mis en jeu dans des expériences de magnétotransport. Une seconde série de calculs portera sur les jonctions de type Fe(100)/Co(bcc)/MgO/Fe(100) ou Fe(100)/Co(bcc)/MgO/Co(bcc)/Fe(100). L'intercalation d'une couche ultra mince de Co épitaxiée permet d'envisager l'existence d'états de puits quantiques dans la couche mince de cobalt, le nombre et l'énergie de ces états dépendant de la largeur de la couche de cobalt. Ces états localisés entre l'électrode de fer et la barrière isolante devraient modifier les propriétés de transport d'une façon que l'on pourra ajuster en modifiant l'épaisseur de la couche de cobalt (et donc le nombre d'états de puits quantique occupés et inoccupés des électrons de spin majoritaire et minoritaire). •Structure fine au seuil L23 des métaux de transition dans les jonctions « Métal 3d/MgO/Métal 3d »: L'étude de la structure fine des spectres EELS

au seuil L23 des métaux de transition concernera les jonctions tunnel Fe/MgO/Fe et FeCo/MgO/FeCo. Il s'agira par exemple de calculer le moment magnétique des atomes au voisinage des interfaces (en tenant éventuellement compte de la présence d'une couche d'oxyde) et de relier la valeur de ce moment magnétique au rapport d'intensité I(L3)/I(L2) mesuré près de l'interface par spectroscopie de pertes d'énergie d'électrons. Remarque: un chercheur post-doc financé par l\'ANR viendra compléter cette équipe en cours d\'année.

Dernières publications:

- PHYSICAL REVIEW B 90, 45411 (2014) -
- JOURNAL OF PHYSICS-CONDENSED MATTER 25, 256002 (2013) -

Propriétés physico-chimiques de nanostructures à base de carbone et autres matériaux 2D: fonctionnalisation et effets d'environnement

Projet démarré en 2008

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Iann Gerber**The design of innovative materials based on nano materials requires a thorough understanding of the physics and chemistry at the atomic scale. The study by DFT calculations of the physico-chemical properties of carbon-based nanostructures has become almost an inescapable fact in many case studies. Indeed it is a major issue to understand complex phenomena related to the functionalization, the doping, the effects of external stress which can be mechanical, electrical or even imposed by a substrate. All this, with future applications in nanocatalysis, or to improve electronic transport properties, or even for a more fundamental understanding of the nature of metal-carbon interactions. Besides, lamellar dichalcogenide based materials have unique physical properties that offer a new field of investigations in optoelectronic mainly. Electronic band structure calculations beyond standard DFT are essential in this study in order to understand photoluminescence experiments.

Dernières publications:

- Carbon 145, 10 (2019) - **doi:** pu.doi
- Catal. Sci. Technol. (2019) - **doi:** pu.doi

Interstitial-solute interactions in metals by numerical simulations, implications on materials' properties: diffusion, cohesion and plasticity

Projet démarré en 2007

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)

Porteur de projet: **Damien Connétable**

The context of the project is the damaging of metallic alloys in their environment. We want to predict, on the long term, the loss of mechanical properties of structural materials (nickel based alloys, steels and aluminum alloys) due to Stress Corrosion Cracking (SCC), hydrogen embrittlement, metal dusting or internal oxidations. The goal of this project is to enhance applications' safety (air plane, civilian nuclear plants, pipelines...) and to reduce maintenance costs. The project consist in the development of a multi-scale simulation (coupling first-principles calculations –DFT- and classical modeling of diffusion processes via Molecular Dynamics, Monte Carlo and explicit equations) of some key mechanisms involved in metallic embrittlement. We will focus on the interactions between interstitials and crystalline defects in metallic systems: point defects, dislocations, interfaces and solutes.

Dernières publications:

- First-principles study of the insertion and diffusion of interstitial atoms (H, C, N and O) in nickel - **doi:** pu.doi
- Theoretical study of oxygen insertion and diffusivity in the g-TiAl L1 0 system - **doi:** pu.doi

Modélisation des nano-structures moléculaires auto-assemblées et de la réactivité sur surfaces

Projet démarré en 2006

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Hao Tang**

The spontaneous self-organization of molecules would not only have a very large number of nano-components in a well defined architecture, but also to obtain specific properties related to the geometry of these structures. However, the mechanisms of these self-assembling are not yet totally well understood. In this project we propose to study the molecular nanostructures as two-dimensional whose formation is the result of balance between molecule-molecule interactions and molecule-substrate interactions. In addition, we will also study the electronic and magnetic properties at the interface molecule as well as to understand how these molecular self-assembled monolayers could stabilize some orientations during the growth of nanoparticles. To do this, we use both quantum methods (DFT, semi-empirical) and classical methods (molecular mechanics, molecular dynamics).

Dernières publications:

- Stepwise on-surface dissymmetric reaction to construct binodal organometallic network. Jing Liu, Qiwei Chen, Kang Cai, Jie Li, Yaru Li, Xiao Yang, Yajie Zhang, Yongfeng Wang, Hao Tang, Dahui Zhao, Kai Wu, Nature Communication, 10, 2545 (2019). - **doi:** pu.doi
- Control of the deprotonation of terephthalic acid assemblies on Ag(111) studied by DFT calculations and low temperature scanning tunneling microscopy. Jeanne Heintz, Corentin Durand, Hao Tang, Roland Coratger, Phys. Chem. Chem. Phys., 2019, DOI:10.1039/C9CP05151A. - **doi:** pu.doi

Simulations de systèmes quantiques fortement corrélés : propriétés magnétiques, supraconductrices et influence du désordre

Projet démarré en 2006

LPT - Laboratoire de Physique Théorique (UMR 5152)

Porteur de projet: **Fabien Alet**

This project is an ongoing continuation (started about 10 years ago) of our scientific activity, located in the field of theoretical condensed matter physics. We deal with physical problems at the quantum electronic scale, where interactions between electrons are very strong, resulting in new physical phenomena. Technically, this is the N-body quantum problem plagued with an exponential complexity. The range of applications of our research is quite broad, from quantum magnets, high-temperature superconductors, ultra-cold atomic systems to quantum localization phenomena. As there is no otherwise general analytical solution, we treat the N-body quantum problem with numerical simulations. Over the years, our group (~ 8 persons) has developed a strong reputation for the development and applications of sophisticated algorithms to fight the underlying exponential complexity: exact diagonalization (ED) including world-wide state of the art algorithms, methods based on Matrix Product States, or quantum Monte Carlo sampling. We have developped algorithms that all use efficient parallelization, with MPI, openMP or hybrid codes. We continue our activity this year, with 3 different directions: 1) Thermodynamics of frustrated magnets, with quantum typicality method 2) Continuing projects on Many-Body Localization, an important research directions since about 4 years. 3) Prospective project on random quantum circuits

Dernières publications:

- Hilbert Space Fragmentation and Many-Body Localization, Francesca Pietracaprina, Nicolas Laflorencie - **url:** pu.open_url
- Multiple Magnetic Bilayers and Unconventional Criticality without Frustration in BaCuSi2O6, S Allenspach, A Biffin, U Stuhr, GS Tucker, S Ohira-Kawamura, M Kofu, DJ Voneshen, M Boehm, B Normand, N Laflorencie, F Mila, Ch Ruegg - **url:** pu.open_url

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4.8 Méthodes et algorithmes

AMAS4BigData

Projet démarré en 2019

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)

Porteur de projet: **Jean-Pierre Georgé**

The objective if to test the "AMAS4BigData" framework, which was developed during a PhD thesis, on scaled-up test cases. This project uses a collective artificial intelligence that analyses, dynamically and in real-time, relations between data sources.

Modélisation de covariances d'erreur d'ébauche sur grille non-structurée

Projet démarré en 2019

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)

Porteur de projet: **Benjamin MENETRIER**

Data assimilation is a set of methods whose goal is to initialize numerical prediction models. These methods usually combine pieces of information from a background (recent forecast) and from observations of the system, weighted according to their respective uncertainty. This uncertainty is represented by error covariance matrices. Because of the system size (often over a billion variables), the background error covariance matrices cannot be explicitly estimated and stored, and have to be modeled. The growing diversity of grids used for numerical modelling of weather, ocean and other compartment of the Earth system requires the development of innovating approaches to model background error covariances on unstructured grids. It is precisely the goal of the BUMP software (Background error covariance on Unstructured Mesh Package), developed by IRIT, Météo-France and the JCSDA (Joint Center for Satellite Data Assimilation, USA). This code is interfaced in the OOPS environment (Object-Oriented Prediction System), developed by ECMWF (European Center for Medium Range Weather Forecast, UK), Météo-France and the JCSDA. OOPS is a flexible tool to develop data assimilation algorithms, test them and use them for operational production. An important aspect of background error covariance modelling is the efficiency and the scalability of the code on massively parallel supercomputers. Indeed, the numerical models resolution increase and the strict time constraints of operational production require an efficient parallelization. The aim of this project is to test the scalability of BUMP algorithms and to compare their performances with other existing methods.

Aging, Entrepreneurship and Frictions in Buying and Selling Activities

Projet démarré en 2019

TSE-R - TSE-R UMR 5314

Porteur de projet: **Sumudu Kankanamge**

This project studies the implications of the aging of entrepreneurs when older individuals have to sell their firms in order to retire. Our first contribution is providing new empirical evidences on business acquisitions and sales using the SSBF, SBO and PSID datasets. We also provide evidence on the important frictions on the business sale market faced by entrepreneurs using a novel dataset. We then build a life-cycle general equilibrium model supporting the above evidence and that combines: (i) occupational choices, (ii) acquisition choices and (iii) business sale market frictions. First calibrated to the US economy, we evaluate the implications of a demographic shock consistent with the retiring baby-boomers. We notably argue that old entrepreneurs will face considerable difficulties in selling their firm to the younger generations, which might generate important economic losses and job destructions. This project is computationally intensive. It requires the calibration and estimation of the model a large number of times.

Dernières publications:

- Young, Eric R., "Solving the incomplete markets model with aggregate uncertainty using the Krusell-Smith algorithm and non-stochastic simulations," Journal of Economic Dynamics and Control, - **doi:** pu.doi **url:** pu.open_url
- Carroll "The method of endogenous gridpoints for solving dynamic stochastic optimization problems" - Economics Letters - **doi:** pu.doi **url:** pu.open_url

Calculs de couverture mobile pour la région Occitanie

Projet démarré en 2019

SGAR31 - SGAR Occitanie

Porteur de projet: **Louis Voisine**

Dans le cadre de l'OpenData et de l'ouverture des données publiques concernant la résorption des zones blanches, nous souhaitons fournir aux différents acteurs des cartes représentant la couverture réelle des locaux et ce, pour tous les opérateurs. Pour cela, nous avons besoin de comparer des cartes de couverture (polygones au format shapefile) avec des coordonnées de locaux afin de déterminer le taux de couverture des communes de la région. L'objectif final de ce projet est de pouvoir utiliser les données en sortie pour des applications de visualisation de données afin de les présenter de la meilleure façon possible. Nous avons besoin de puissance pour faire tourner ces calculs lourds pour accélérer le processus (plusieurs millions de polygones et plusieurs centaines de milliers de locaux pour la région).

Homogenization theory and numerical approaches applied to mortar using waste aggregates: study of its mechanical behavior and durability

Projet démarré en 2019

LMDC - Laboratoire Matériaux et Durabilité des Constructions de Toulouse

Porteur de projet: **Ariane Abou Chakra**

For many years, researches are devoted to improve concrete material to obtain better performances and durability, we can refer to High-performance concrete (HPC) and Ultra-high-performance concrete (UHPC). This manufacturing material is one of the most widely used building materials in the world. It is an attractive artificial composite material which can obtain very attractive performances for the building industry needs. On the other hand, it appears that concrete is a polluting material. Concrete industry which has cost a lot of energy consumption and resources is confronted with the challenges of reducing the CO2 emission. Moreover, intensive exploitation of aggregates rock in concrete creates environmental problems as depletion of natural resources. Whereas cities

needs more and more concrete production, we produce more and more waste. Incorporating waste aggregates into concrete would both divert them from landfills and reduce our CO2 emissions. The research topic presented here is thus part of the problematic of replacement of natural resources by a recycled and recycled post-consumer product. So, the proposed research project has for main objective the understanding of the impact of recycled particles in concrete on the mechanical behavior and its durability. Research work plan: 1. Mechanical predictions of mortar containing recycled waste: theoretical micromechanical modeling of the behavior and finite element approach using a representative volume elementary (RVE) 2. Micromechanical approaches to predict the durability

Deep learning for classifying histopathological images: application to cancer diagnosis

Projet démarré en 2019

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)

Porteur de projet: **MD ZIA ULLAH**

Recently, deep learning has attracted a lot of attention to model the multimodal and multi-resolution medical images, due to its state of the art performance in image recognition, machine translation, etc. The automated diagnosis of cancer from histopathological images is an interesting problem from both machine learning and medical practitioner community. Diagnosis refers to the characterizing, detecting, and localizing the pathological patterns of the medical data. Each histopathological image possesses a set of multi-resolution layers with complementary information; deep learning tool would leverage this diverse information to learn an ensemble model. The deep learning model lacks the confidence of prediction that is essential for a cancer diagnosis; our objective is to estimate the confidence of deep learning model from deep architecture. To evaluate our objectives, we would like to access your invaluable resources.

LUDAU

Projet démarré en 2019

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)

Porteur de projet: **Thomas Pellegrini**

Dans le cadre de mon projet ANR LUDAU sur le deep learning appliqué à l'analyse de contenus sonores (reconnaissance vocale, détection d'événements sonores), nous avons besoin de capacités de calcul sur GPU e plus en plus importantes. Jusqu'à présent nous avons utilisé OSIRIM et nous continuerons à le faire, cependant les réseaux de neurones et les datasets associés sont de plus en plus gros. CALMIP devrait nous permettre de passer à l'échelle plus facilement.

ECHOPPE, Economie du logement

Projet démarré en 2018

TSE-R - TSE-R UMR 5314

Porteur de projet: **celine parzani**

Housing is a critical target of public policy in France. The budget of housing policies devoted to transfers exceeded 40 billion euros in 2014 or approximately 2% of GDP. These policies include housing benefits, property taxes and construction subsidies and extend to social housing and rent controls. The goal of this project is to build up dynamic structural models of household inter-temporal decisions regarding their housing with an emphasis on life-cycle issues, and to calibrate these models using French data. There exists no such empirical model for France

and only recently for the US. This core model will be used to assess the long-run impacts of housing public policies like housing benefits, means-tested zero-interest loans to first time owners etc. In particular, it would measure the order of magnitude of the reduction of housing inequalities that can be achieved by public policies, including general equilibrium effects through prices and rents. To do so, we consider a model in which households, who are stochastically ageing and changing their marginal productivity, choose, each year, whether to rent or to buy their house (or another one to rent it to other households), to consume and to save . A parametric utility function is assumed and there are institutional constraints added to the model : the tax system faced by the households and the borrowing constraints. The goal is to first estimate the value function of a given household which depends on its earnings, his wealth, his housing situation and, of course, on the parameters of the model. Once this value function is determined, we need to estimate the renting price and housing price by balancing the two sides of the markets (supply and demand). Ultimately, we aim at estimating the utility parameters by comparing some aggregate statistics estimated on the French Housing Survey and predicted by our model. The final results will be used for counterfactual analysis.

Algorithmes parallèles pour la résolution de problèmes issus de la discrétisation d'équations aux dérivées partielles

Projet démarré en 2017

ISAE/DISC - Département d'Ingénierie des Systèmes Complexes

Porteur de projet: **Xavier Vasseur**

Efficient parallel algorithms for the numerical solution of partial differential equations are required for solving large-scale problems in Computational Science and Engineering. This project aims at tackling certain aspects of modern methods for the solution of nonlinear systems issued from the discretization of partial differential equations. We focus on the analysis and implementation of algorithms for the model reduction of dynamical systems coming from the discretization of time-dependent partial differential equations. We plan to investigate the potential of recent algorithms based on randomized linear algebra in such a context. We aim at proposing an implementation of such randomized algorithms in Julia to exploit both the native parallelism of Julia and the GPU capabilities of Olympe.

Dernières publications:

- T. Lunet, J. Bodart, S. Gratton and X. Vasseur "Time-parallel simulation of the decay of homogeneous turbulence using Parareal with spatial coarsening". Comput. Vis. Sci., 19-1–2, pp. 31–44, 2018. - **doi:** pu.doi **url:** pu.open_url
- T. Lunet, Stratégies de parallélisation espace-temps pour la simulation des écoulements turbulents, Thèse de doctorat, ISAE-SUPAERO, thèse soutenue le 9 janvier 2018. - **url:** pu.open_url

Fast Kinetic Schemes for Boltzmann equation

Projet démarré en 2017

IMT - Institut de Mathématiques de Toulouse (UMR 5219)

Porteur de projet: **Jacek Narski**

The aim of the project is to develop an efficient parallel algorithm to perform deterministic numerical simulations of the rarefied gas dynamics on distributed memory systems. The rarefied gas dynamics described by a full Boltzmann equation defined in 7D (three coordinates in the physical space, three coordinates in the velocity space and time). The numerical scheme that is considered is an extension of the Fast Kinetic Scheme (FKS) [J. Comput. Phys., Vol. 255, 2013, pp 680-698] originally constructed for solving the BGK equation, to the more challenging

case of the Boltzmann equation, where the collisions between particles are modeled by multiple integrals over the whole velocity space. The scheme combines a robust and fast method for treating the transport part based on an innovative Lagrangian technique supplemented with fast spectral schemes to treat the collisional operator by means of an operator splitting approach. The construction of the FKS makes it extremely well suited for parallelization on shared or distributed memory systems. The OpenMP and GPU parallization was the objective of a previous work [J. Comput. Phys., Vol. 284, 2015, pp 22-39]. The strong scaling obtained was close to ideal. However, due to the curse of dimensionality of the Boltzmann equation, the size of the problems that can be treated on a shared memory systems is very limited. The necessary next step is to move beyond shared memory system to distributed systems. The approach that is choosen for parallelization is the decomposition of the physical space: every computational node contains only a subset of the physical domain and a whole velocity space. This strategy allows to evaluate the Boltzmann collision operator (multiple integral over the velocity space) without any additional MPI communication required. Finally, computations on every node are performed in parallel using the OpenMP framework.

Dernières publications:

- Jacek Narski, Fast Kinetic Scheme: efficient MPI parallelization strategy for 3D Boltzmann equation, Commun. Comput. Phys., 25 (2019), pp. 361-389 - **doi:** pu.doi

Modelisation THCM des ouvrages en béton, béton armé et précontraint

Projet démarré en 2016

LMDC - Laboratoire Matériaux et Durabilité des Constructions de Toulouse

Porteur de projet: **Laurie Lacarriere**

The main objective of this project is to study the thermo-hydro-chemo-mechanical (THCM) behavior of concrete and reinforced concrete structures (confinement vessels, larges beams of bridges). The coupling between physico-chemical and mechanical behavior is studied for several applications (early age, ageing concrete, severe accident with high temperatures, chemical endogenous attack, ...).

Embryogenèse de créatures et de réseaux de neurones artificiels

Projet démarré en 2016

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)

Porteur de projet: **Sylvain Cussat-blanc**

Artificial embryogenesis aims to mimic or to take inspiration from the natural process of embryogenesis either to generate artificial creatures that populate virtual worlds or to simulate cell proliferation for biological matters. Embryogenesis is the process that grows a living being from a unique egg cell. This process implies extremely complex mechanisms such as cell division and cell specialization both orchestrated by genetic regulation. The aim of this project is to develop in-silico models of artificial embryogenesis, also named a evo-devo model, that simulate the cell in its chemical and/or physical environment and its internal control via an evolved artificial gene regulatory network. This latter generates the behavior of the cells: as in nature, by sensing the protein concentration of its direct neighborhood and inside its own membrane, the cell can decide between dividing, specializing, waiting for better environmental condition (quiescence), committing a suicide (apoptosis) or migrate. With these models, multiple objectives will be addressed. First, this model can be used to produce artificial creatures by evolving (with a genetic algorithm for example) the gene regulatory network of the cell. This allows the study of the evolutionary process of multicellular organisms under particular environmental conditions.

Another goal of this model is to simulate the growth of neural networks in order to produce larger, scalable and adaptative behavior engines to control virtual robots in complex changing environments.

Dernières publications:

- Learning Aquatic Locomotion for Animats -
- A Comparison of Genetic Regulatory Network Dynamics and Encoding -

Algèbre Linéaire Creuse (MUMPS, Méthodes Hybrides)

Projet démarré en 2009

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)

Porteur de projet: **Patrick Amestoy**

Our project focusses on sparse parallel algorithms, more precisely on the parallel solution of large sparse linear systems based on both direct and hybrid methods (mixing direct and iterative methods). Our work can impact the performance of many applications, in particular simulations using finite element or finite difference methods as well as numerical optimization problems. Two main aspects of our research are the scalability of our methods on problems with millions of equations when increasing the number of processors and the use of so called block low rank approximation techniques to reduce both memory and floating point number complexity of our algorithms. To reduce the memory and flops complexity we are also investigating hybrid methods based on block Cimmino approach. Our project takes place in the context of a strong collaboration between IRIT (APO team), LaBRI, LIP (Team ROMA) and CERFACS (through a joint lab with IRIT). On real large 3D problems of size few hundred million variables we want to analyse the potential and limit of both direct approaches and hybrid resolution methods. Our work is often based on one of the following software research platforms: http://mumps.enseeiht.fr http://buttari.perso.enseeiht.fr/qr_mumps/ http://abcd.enseeiht.fr/ All software are freely distributed and the improvement of the parallel behaviour of our solvers has a direct benefit for the scientific community.

Dernières publications:

- P.R. Amestoy, A. Buttari, J-Y. L'Excellent & T. Mary, Bridging the Gap between Flat and Hierarchical Low-rank Matrix Formats in SIAM Conference on Computational Science and Engineering (SIAM CSE'19), Spokane, USA, February 2019. - **url:** pu.open_url
- S. Mouysset and R. Guivarch. Parkerc : Toolbox for parallel kernel clustering me- thods. In Proceedings of International Conference on Pattern Recognition Systems, Tours (France), 8-10 July 2019, ISBN 978-1-83953-108-8, pages 82–87, 2019. -